

# **Sentaurus™ Process User Guide**

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**SYNOPSYS®**

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# About This Guide

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The Synopsys Sentaurus™ Process tool is an advanced 1D, 2D, and 3D process simulator suitable for silicon and nonsilicon semiconductor devices. It features modern software architecture and state-of-the-art models to address current and future process technologies.

Sentaurus Process simulates all standard process simulation steps, diffusion, analytic implantation, Monte Carlo implantation, oxidation, etching, deposition, and silicidation. Three-dimensional capabilities include meshing of 3D boundary files using the MGOALS module, mechanics (stress and strain), diffusion, a limited capability for 3D oxidation, and an interface to Sentaurus Structure Editor, which is the 3D geometry editing tool based on the ACIS solid modeling library.

Sentaurus Process uses the Alagator scripting language that allows users to solve their own diffusion equations. Alagator can be used to solve any diffusion equation including dopant, defect, impurity, and oxidant diffusion equations. Simulation of 3D diffusion is handled exactly as for 1D and 2D. Therefore, all the advanced models and user programmability available in 1D and 2D can be used in 3D. In addition, a set of built-in calibrated parameters is available with Advanced Calibration.

---

## Related Publications

For additional information, see:

- The TCAD Sentaurus release notes, available on the Synopsys SolvNet® support site (see [Accessing SolvNet on page xxxii](#)).
- Documentation available on SolvNet at <https://solvnet.synopsys.com/DocsOnWeb>.

---

## Conventions

The following conventions are used in Synopsys documentation.

Convention	Description
Blue text	Identifies a cross-reference (only on the screen).
<b>Bold text</b>	Identifies a selectable icon, button, menu, or tab. It also indicates the name of a field or an option.
Courier font	Identifies text that is displayed on the screen or that the user must type. It identifies the names of files, directories, paths, parameters, keywords, and variables.

Convention	Description
<i>Italicized text</i>	Used for emphasis, the titles of books and journals, and non-English words. It also identifies components of an equation or a formula, a placeholder, or an identifier.
<b>Menu &gt; Command</b>	Indicates a menu command, for example, <b>File &gt; New</b> (from the <b>File</b> menu, select <b>New</b> ).

---

## Customer Support

Customer support is available through the Synopsys SolvNet customer support website and by contacting the Synopsys support center.

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### Accessing SolvNet

The SolvNet support site includes an electronic knowledge base of technical articles and answers to frequently asked questions about Synopsys tools. The site also gives you access to a wide range of Synopsys online services, which include downloading software, viewing documentation, and entering a call to the Support Center.

To access the SolvNet site:

1. Go to the web page at <https://solvnet.synopsys.com>.
2. If prompted, enter your user name and password. (If you do not have a Synopsys user name and password, follow the instructions to register.)

If you need help using the site, click **Help** on the menu bar.

---

### Contacting Synopsys Support

If you have problems, questions, or suggestions, you can contact Synopsys support in the following ways:

- Go to the Synopsys [Global Support Centers](#) site on synopsys.com. There you can find e-mail addresses and telephone numbers for Synopsys support centers throughout the world.
- Go to either the Synopsys SolvNet site or the Synopsys Global Support Centers site and [open a case online](#) (Synopsys user name and password required).

## Contacting Your Local TCAD Support Team Directly

Send an e-mail message to:

- support-tcad-us@synopsys.com from within North America and South America.
  - support-tcad-eu@synopsys.com from within Europe.
  - support-tcad-ap@synopsys.com from within Asia Pacific (China, Taiwan, Singapore, Malaysia, India, Australia).
  - support-tcad-kr@synopsys.com from Korea.
  - support-tcad-jp@synopsys.com from Japan.
- 

## Acknowledgments

Sentaurus Process is based on the 2000 and 2002 releases of FLOOPS written by Professor Mark Law and coworkers at the University of Florida. Synopsys acknowledges the contribution of Professor Law and his advice in the development of Sentaurus Process. Go to <http://swamp.mse.ufl.edu/> for more information about TCAD at the University of Florida.

Sentaurus Process Kinetic Monte Carlo is based on DADOS written by Professor Martin Jaraiz and coworkers at the University of Valladolid, Spain. Synopsys acknowledges Professor Jaraiz' contribution and advice.

## **About This Guide**

Acknowledgments

*This chapter provides an overview of the functionality of Sentaurus Process and describes how to start the tool.*

The TCAD Sentaurus Tutorial provides a range of projects to assist users to work with the tool. To access the tutorial, go to:

```
$STROOT/tcad/$STRELEASE/Sentaurus_Training/index.html
```

where `STROOT` is an environment variable that indicates where the Synopsys TCAD distribution has been installed, and `STRELEASE` indicates the Synopsys TCAD release number.

---

## Overview

Sentaurus Process is a complete and highly flexible, multidimensional, process modeling environment. With its modern software architecture and extensive breadth of capabilities, Sentaurus Process is a state-of-the-art process simulation tool. Calibrated to a wide range of the latest experimental data using proven calibration methodology, Sentaurus Process offers unique predictive capabilities for modern silicon and nonsilicon technologies.

Sentaurus Process accepts as input a sequence of commands that is either entered from standard input (that is, at the command prompt) or composed in a command file. A process flow is simulated by issuing a sequence of commands that corresponds to the individual process steps. In addition, several commands allow you to select physical models and parameters, grid strategies, and graphical output preferences, if required. You should place parameter settings in a separate file, which is sourced at the beginning of command files using the `source` command.

In addition, the Alagator scripting language allows you to describe and implement your own models.

---

## Setting Up the Environment

The `STROOT` environment variable is the TCAD Sentaurus root directory, and you must set this variable to the installation directory of TCAD Sentaurus. The `STRELEASE` environment variable can be used to specify the release of the software to run, for example, N-2017.09. If `STRELEASE` is not set, the default version is used which is usually the last version installed.

## 1: Getting Started

### Starting Sentaurus Process

To set the environment variables:

1. Set the TCAD Sentaurus root directory environment variable STROOT to the TCAD Sentaurus installation directory, for example:

```
* Add to .cshrc  
  
setenv STROOT <Sentaurus directory>  
  
* Add to .profile, .kshrc, or .bashrc  
  
STROOT=<Sentaurus directory>; export STROOT
```

2. Add the <Sentaurus directory>/bin directory to the user path.

For example:

```
* Add to .cshrc:  
  
set path=(<Sentaurus directory>/bin $path)  
  
* Add to .profile, .kshrc, or .bashrc:  
  
PATH=<Sentaurus directory>/bin:$PATH  
export PATH
```

---

## Starting Sentaurus Process

You can run Sentaurus Process in either interactive mode or batch mode. In interactive mode, a whole process flow can be simulated by entering commands line-by-line as standard input. To start Sentaurus Process in interactive mode, enter the following on the command line:

```
> sprocess
```

Sentaurus Process displays version and host information, followed by the Sentaurus Process command prompt. You now can enter Sentaurus Process commands at the prompt:

```
sprocess>
```

This is a flexible way of working with Sentaurus Process to test individual process steps or short sequences, but it is inconvenient for long process flows. It is more useful to compile the command sequence in a command file, which can be run in batch mode or inside Sentaurus Workbench.

To run Sentaurus Process in batch mode, load a command file when starting Sentaurus Process, for example:

```
> sprocess input.cmd
```

---

## Starting Different Versions of Sentaurus Process

To list all available releases in the TCAD Sentaurus installation directory, enter:

```
> sprocess -releases
```

To list all versions in a particular release directory, enter:

```
> sprocess -versions
```

You can select a specific release and version number of Sentaurus Process using the `-rel` and `-ver` options as follows:

```
> sprocess -rel <rel_number> -ver <version_number>
```

For example:

```
> sprocess -rel M-2016.12
```

The following command starts the simulation of `nmos_fps.cmd` using version 1.2 of release M-2016.12 as long as this version is installed:

```
> sprocess -rel M-2016.12 -ver 1.2 nmos_fps.cmd
```

---

## Using a Command File

Instead of entering Sentaurus Process commands line-by-line, the required sequence of commands can be saved to a command file, which can be written entirely by users. To save time and reduce syntax errors, you can copy and edit examples of command files available from the TCAD Sentaurus Tutorial or in this user guide.

If a command file has been prepared, run Sentaurus Process by typing the following command:

```
sprocess <command_filename>
```

Alternatively, you can automatically start Sentaurus Process through the Scheduler in Sentaurus Workbench. The command file has the extension `.cmd`. (This is the convention used in Sentaurus Workbench.)

The command file is checked for correct syntax and then commands are executed in sequence until the simulation is stopped by the command `exit` or the end of the file is reached. Since Sentaurus Process is written as an extension of the tool command language (Tcl), all Tcl commands and functionalities (such as loops, control structures, creating and evaluating variables) are available in command files. This results in some limitations in syntax control if

## 1: Getting Started

### Using a Command File

the command file contains complicated Tcl commands. You can switch off syntax-checking with the command-line option `-n`, for example:

```
sprocess -n commandfile
```

Sentaurus Process ignores character strings starting with a hash (#) character (although Sentaurus Workbench interprets # as a special character for conditional statements). Therefore, this special character can be used to insert comments in the simulation command file.

A file with the extension `.log` is created automatically whenever Sentaurus Process is run from a command line, that is, outside the Sentaurus Workbench environment. This file contains the runtime output, which is generated by Sentaurus Process and is sent to standard output. When Sentaurus Process is run using a command file `<root_filename>_fps.cmd`, the output file is named `<root_filename>_fps.log`.

When Sentaurus Process is run from Sentaurus Workbench, the output file is named `<root_filename>_fps.out`.

For a complete list of commands, see [Appendix A on page 897](#).

*This chapter provides an overview of how Sentaurus Process operates.*

The syntax and features of the command file are described, followed by an overview of the parameter database, which contains all of the model parameters, and technical details regarding the running of the tool.

For new users, see [Interactive Mode on page 12](#), [Syntax for Creating Command Files on page 16](#), and [Creating and Loading Structures and Data on page 39](#). For advanced users who need to adjust model parameters, see [Parameter Database on page 21](#).

---

## Overview

To familiarize users with the different formatting used in this documentation, input commands from either a command file or the command line are presented this way:

```
sprocess -v
```

An example of output is:

```
*****
***                               Sentaurus Process      ***
***                               Version N-2017.09    ***
***                               (1.7, RHEL64)       ***
***                                         ***
***                                         Copyright (C) 1993-2002 ***
***                                         The board of regents of the University of Florida ***
***                                         Copyright (C) 1994-2017   ***
***                                         Synopsys, Inc.        ***
***                                         ***
***   This software and the associated documentation are confidential ***
***   and proprietary to Synopsys, Inc. Your use or disclosure of this ***
***   software is subject to the terms and conditions of a written ***
***   license agreement between you, or your company, and Synopsys, Inc. ***
*****
```

Compiled Fri Jul 14 23:54:02 PDT 2017 on tcadprod8

Started at: Tue Jul 11 10:25:16 2017 (CEST)  
User name: jbrowne

## 2: Working With the Simulator

### Interactive Visualization

```
Host name: topo2
PID: 25333
Architecture: x86_64
Operating system: Linux rel. 2.6.18-274.12.1.el5 ver. #1 SMP Tue Nov 8 21:37:35
EST 2011
```

---

## Interactive Visualization

The options for interactive visualization in Sentaurus Process are:

- An X-Windows-based graphical display (which will be phased out in future releases)  
This viewer can be used for 1D and 2D simulations, and is launched with either the `plot.1d` or `plot.2d` command (see [plot.1d on page 1111](#) and [plot.2d on page 1114](#)).
- An interface to Sentaurus Visual (which will eventually replace the X-Windows display)

---

## Interface to Sentaurus Visual

The interface to Sentaurus Visual can visualize 1D, 2D, and 3D structures and data evolution while the simulation progresses (see [Figure 1 on page 7](#)). The interface is initiated and controlled from Sentaurus Visual, including control of the simulation.

Table 1 Buttons of the Simulation Control panel of Sentaurus Visual

Button	Description
	Load: Load a command file. When a command file is loaded, it is thereafter referred to as the <i>flow</i> .
	Run: Run the flow. Use this button either to start running the flow or to continue execution after pausing the flow. The simulation continues at the location of the cursor (line with a light-yellow background).
	Pause: Pause the running flow. The pause occurs either when the currently executing step (command) is finished or, for a long-running step, when the current time step is completed.
	Reset: Reset the running flow. The running flow stops, the connection to the simulator is terminated, and you return to the start of the flow.
	Run Step: Run the next step in the flow. When you click this button, either a single step (command) is executed or a group of commands enclosed in braces is executed. You must repeatedly click this button to execute the next steps.

Table 1 Buttons of the Simulation Control panel of Sentaurus Visual

Button	Description
	Save: Save the flow.
	Save As: Save the flow under a new name.

In addition, the `graphics` command can be used to control the plot settings in Sentaurus Visual and to select which fields are visible (see [graphics on page 970](#)).

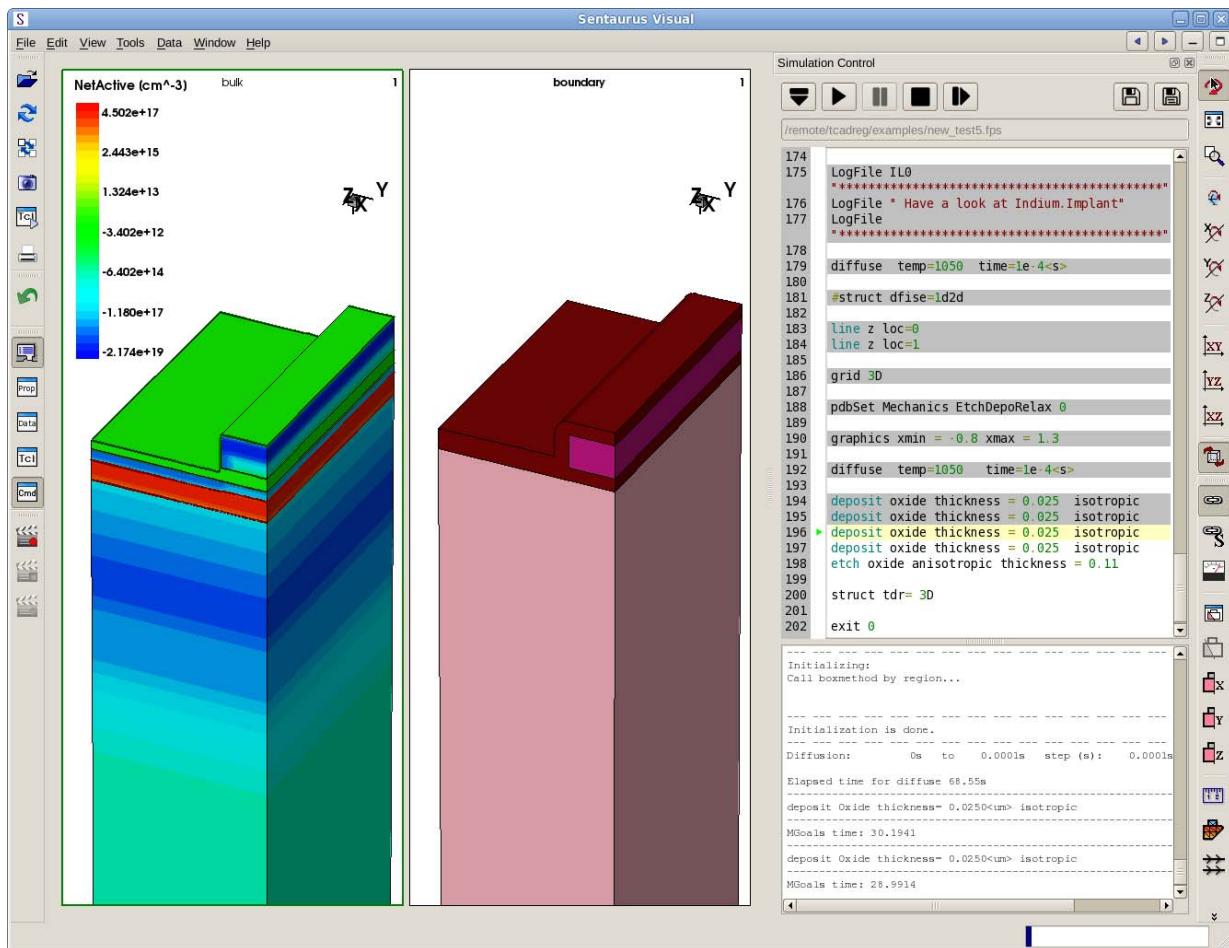


Figure 1 Interface to Sentaurus Visual: upper pane of Simulation Control panel shows command file and lower pane of Simulation Control panel shows log file

## 2: Working With the Simulator

### Interactive Visualization

## Setting Up the Interface

To set up and to run the interface:

1. Launch Sentaurus Visual with the following command-line options:

```
> svisual -spi &
```

2. In Sentaurus Visual, choose **Edit > Preferences**.
3. In the User Preferences dialog box, expand the categories to **Common > Miscellaneous**.
4. In the Simulator group box:
  - a) In the **Command** field, type the tool binary as well as any command-line option required, for example:  

```
sprocess -n
```
  - b) In the **Communication Option** field, type `--svi`.
5. Click **Save**.

## Loading Command Files

To load a command file:

1. In the Simulation Control panel, click the Load button (see [Figure 1 on page 7](#)).  
The Load File dialog box is displayed.
2. Select the command file to open.
3. Click **Open**.

In addition, a command file can be loaded from the command line using:

```
svisual -spi <filename>
```

## Inserting Breakpoints in the Flow

To set breakpoints to pause the simulation at a particular step in the flow:

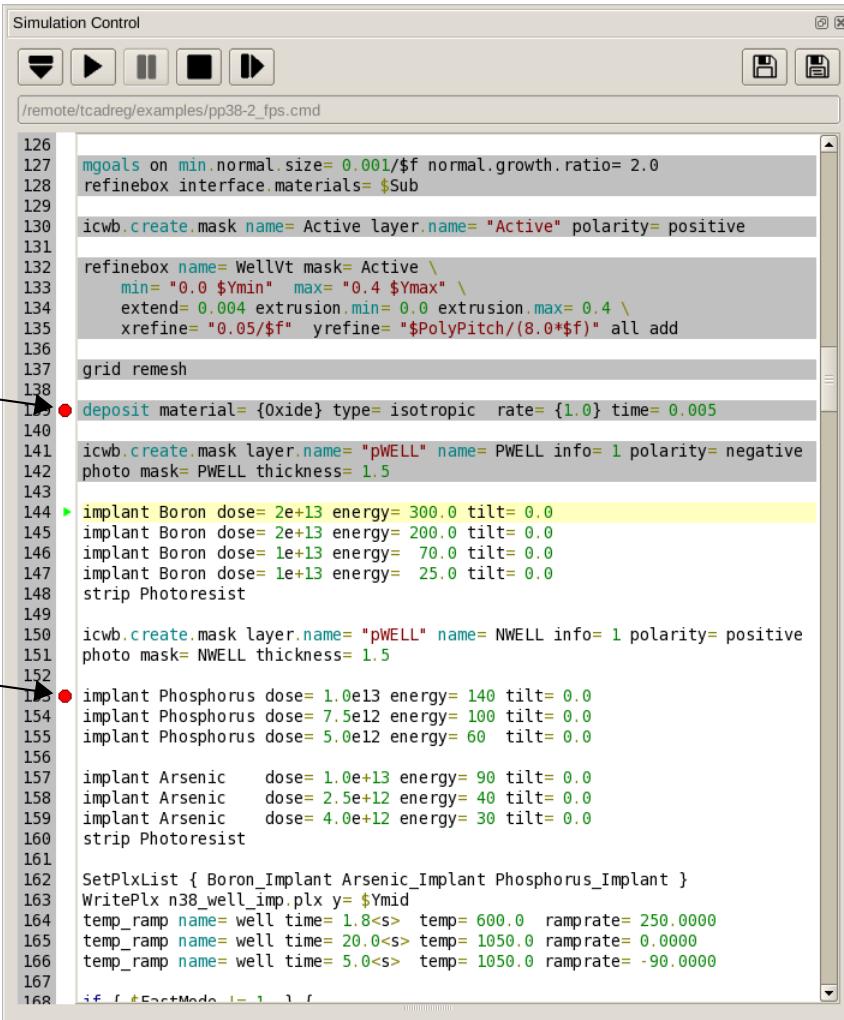
1. Click in the left margin, at the line corresponding to the step (command) where you want the flow to stop.  
A red circle marks the breakpoint (see [Figure 2 on page 9](#)).
2. Click the **Run** button to execute the entire flow or the Run Step button to execute individual steps.

**NOTE** You can set multiple breakpoints in a flow.

## Deleting Breakpoints in the Flow

To delete a breakpoint:

- Click the red circle in the left margin.



The screenshot shows the 'Simulation Control' window with a command-line interface. The window title is 'Simulation Control'. The menu bar includes 'File', 'Edit', 'Run', 'Help', and 'About'. Below the menu is a toolbar with icons for opening, saving, running, and stopping. The main area is a text editor displaying a command script. The script content is as follows:

```

126 mgoals on min_normal.size= 0.001$f normal.growth.ratio= 2.0
127 refinebox interface.materials= $Sub
128
129 icwb.create.mask name= Active layer.name= "Active" polarity= positive
130
131 refinebox name= WellVT mask= Active \
132     min= "0.0 $Ymin" max= "0.4 $Ymax" \
133     extend= 0.004 extrusion.min= 0.0 extrusion.max= 0.4 \
134     xrefine= "0.05/$f" yrefine= "$PolyPitch/(8.0*$f)" all add
135
136 grid remesh
137
138 deposit material= {Oxide} type= isotropic rate= {1.0} time= 0.005
139
140 icwb.create.mask layer.name= "pWELL" name= PWELL info= 1 polarity= negative
141 photo mask= PWELL thickness= 1.5
142
143 > implant Boron dose= 2e+13 energy= 300.0 tilt= 0.0
144 implant Boron dose= 2e+13 energy= 200.0 tilt= 0.0
145 implant Boron dose= 1e+13 energy= 70.0 tilt= 0.0
146 implant Boron dose= 1e+13 energy= 25.0 tilt= 0.0
147 strip Photoresist
148
149 icwb.create.mask layer.name= "pWELL" name= NWELL info= 1 polarity= positive
150 photo mask= NWELL thickness= 1.5
151
152 > implant Phosphorus dose= 1.0e13 energy= 140 tilt= 0.0
153 implant Phosphorus dose= 7.5e12 energy= 100 tilt= 0.0
154 implant Phosphorus dose= 5.0e12 energy= 60 tilt= 0.0
155
156 implant Arsenic dose= 1.0e+13 energy= 90 tilt= 0.0
157 implant Arsenic dose= 2.5e+12 energy= 40 tilt= 0.0
158 implant Arsenic dose= 4.0e+12 energy= 30 tilt= 0.0
159 strip Photoresist
160
161 SetPlxList { Boron_Implant Arsenic_Implant Phosphorus_Implant }
162 WritePlx n38_well_imp.plx y= $Ymid
163 temp_ramp name= well time= 1.8<s> temp= 600.0 ramprate= 250.0000
164 temp_ramp name= well time= 20.0<s> temp= 1050.0 ramprate= 0.0000
165 temp_ramp name= well time= 5.0<s> temp= 1050.0 ramprate= -90.0000
166
167 if f & FastMode l= 1 1
168

```

Two specific lines in the script are highlighted with yellow backgrounds and marked with red circles in the left margin, indicating they are breakpoints. The first highlighted line is 'deposit material= {Oxide} type= isotropic rate= {1.0} time= 0.005' at line 138. The second highlighted line is 'implant Phosphorus dose= 1.0e13 energy= 140 tilt= 0.0' at line 152.

Figure 2 Setting a breakpoint in the flow (red circle indicates location of breakpoint)

## Indicating Status of Steps

In the Simulation Control panel, as the flow is being executed, a green triangle in the left margin (in the same location as breakpoints) indicates the step that will be executed next. A red triangle indicates the step that is currently being executed.

## 2: Working With the Simulator

### Interactive Visualization

Already executed steps are indicated with a gray background. This part of the flow cannot be changed further.

In addition, wherever the cursor is in the flow, its position is indicated by highlighting the line with a light yellow background.

## Updating the Structure

In 3D simulations, two plots are shown with the titles ‘bulk’ and ‘boundary’ (see [Figure 1 on page 7](#)). This is because, in 3D simulations, both the bulk and boundary are not always up to date. The plot with its title in bold shows the last updated information. For example, if the `insert` command is called in a 3D simulation, the boundary is updated; however, by default, the mesh is not updated. After the insertion operation is completed, the title of the ‘boundary’ plot will be bold, and the title of the ‘bulk’ plot will not be bold.

---

## Controlling the Interface to Sentaurus Visual With the graphics Command

To quickly visualize the evolution of a structure or data, the use of the `graphics` command is not necessary. Simply launch the interface to Sentaurus Visual and adjust the plot settings in Sentaurus Visual.

However, when setting up a flow for the first time or for calibration-type activities, the same command file might need to be run and rerun many times. In these cases, it is convenient to use the `graphics` command to specify the Sentaurus Visual plot settings directly into the command file to avoid having to repeatedly change the plot settings in Sentaurus Visual for each run.

Another case where the `graphics` command is needed is choosing the availability or selection of nonstandard fields for visualization.

In general, `graphics` commands are executed in the usual sequential order as specified in the command file; whereas, settings specified in Sentaurus Visual will be executed immediately. In either case, the latest command to be executed will determine the current settings.

Unless otherwise specified, the arguments of the `graphics` command are independent and can be used in any combination (see [graphics on page 970](#)).

## Command-Line Options

[Table 2](#) lists the command-line options that are available in Sentaurus Process.

Table 2 Command-line options

Option	Short name of option (if available)	Function
--batchMode	-b	Switches off graphics.
--diff		Diff mode. To see differences in data and Sentaurus Process parameter settings between two TDR files. Interpolation is used to compare results from different meshes. Usage: <code>sprocess --diff &lt;file1&gt; &lt;file2&gt;</code> where <file1> and <file2> are TDR files.
--FastMode	-f	Generates structure, no diffusion, no Monte Carlo implantation, no partial differential equation (PDE) solve, and so on.
--GENESISMode	-u	Switches off log file creation.
--home <directory>	-o <directory>	Sets SPHOME to <directory>.
--noSyntaxCheck	-n	Switches off syntax check.
--pdb	-p	Runs the Parameter Database (PDB) Browser showing parameters as they are set during runtime. Includes default parameters and parameters from the command file if specified.
--ponly		Same as --pdb, but only shows parameters set in the command file; does not show default parameters.
--quickSyntaxCheck	-q	Only checks syntax of branches that are true.
--svi		Switches on the Sentaurus Visual interface mode. This option is usually specified in the User Preferences dialog box of Sentaurus Visual (see <a href="#">Setting Up the Interface on page 8</a> ).
--syntaxCheckOnly	-s	Only checks syntax, no execution.
--xml		Switches on the creation of an XML-style marked-up log file for use in the TCAD Logfile Browser (see <a href="#">Utilities User Guide, Chapter 2 on page 5</a> ).
	-v	Prints header with version number.
	-h	Prints use and command-line options.

## 2: Working With the Simulator

### Command-Line Options

Table 2 Command-line options

Option	Short name of option (if available)	Function
	-x	Tests floating-point exception handling.
	-X	Switches off floating-point exception catching.

---

## Interactive Mode

Sentaurus Process runs in interactive mode if no command file is given. In this mode, commands can be entered (at the command prompt) line-by-line and are executed immediately.

It is useful to run Sentaurus Process in the interactive mode for the following reasons:

- When debugging Tcl code, the program does not quit if a Tcl error is found. The error is displayed and you are prompted again for input. You can source a command file repeatedly if required.
- To easily obtain PDB parameter names and defaults with the `pdbGet` command.
- To print the list of built-in functions with the `help` command, and to print the list of Tcl procedures with the `info procs` command.
- To obtain command parameter names and defaults for any built-in command by using the `params` flag available in all built-in functions.

Another use of the interactive mode is to pause the simulation using the `fbreak` command. When the simulation is paused in interactive mode, the state of the simulator can be queried using a number of commands including `grid`, `mater`, and `select`. Pausing the simulation can also be useful when using interactive graphics as described in [Interactive Visualization on page 6](#).

---

## Fast Mode

When working on a new process flow, it is useful to run Sentaurus Process a few times using the fast mode (-f command-line option). Developing a new process flow can be complex, involving many `etch`, `deposit`, and `photo` steps, some with masks; sometimes adjustments are required. In the fast mode, all diffusion including oxidation, Monte Carlo implantation, and 3D remeshing commands are ignored. Only process commands for structure generation and analysis are performed. In this mode, when in three dimensions, all `struct` commands will write only a boundary into a TDR file, since the simulation mesh is not synchronized with the modified structure.

## Terminating Execution

You can terminate a running Sentaurus Process job in several ways. In some cases, the termination will take time or will fail for other reasons. The most fail-safe method is to use the UNIX command:

```
kill -9 <process_id>
```

where `<process_id>` is the process ID number of the running Sentaurus Process job which can be obtained with the UNIX `ps` command. This sends a signal `SIGKILL` to the corresponding Sentaurus Process job, which will cause the job to terminate immediately.

If Sentaurus Process is run directly from a UNIX shell, usually you can terminate the run by using shortcut keys. The key sequence is interpreted by the shell command, which sends a signal to the job in the foreground. Usually, `Ctrl+C` sends a `SIGINT` signal and `Ctrl+\` (backslash) sends a `SIGQUIT` signal. The running Sentaurus Process job catches all `SIGINT` signals and waits for three signals to be caught (in case it was typed accidentally) before terminating itself.

However, Sentaurus Process does not catch the `SIGQUIT` signal, so this signal will typically cause Sentaurus Process to terminate immediately.

Because the exact behavior may depend on your UNIX shell, the operating system, and the local configuration, refer to the manual for the UNIX shell you are running or contact your local systems administrator for more information.

---

## Environment Variables

The Sentaurus Process binary relies on several supporting files found using the environment variables `SPHOME` and `SCHOME`. To change default models and parameters without modifying the installed Sentaurus Process files, copy the default `SPHOME` and `SCHOME` directories and set the environment variables (`SPHOME` and `SCHOME`) to the location of the modified directories.

By default, `SPHOME` and `SCHOME` are set based on the Synopsys standard environment variables `STROOT` and `STRELEASE`, and by the version number of Sentaurus Process using:

```
SPHOME = $STROOT/tcad/$STRELEASE/lib/sprocess-<version number>
SCHOME = $STROOT/tcad/$STRELEASE/lib/score-<version number>
```

## 2: Working With the Simulator

### File Types

The \$PHOME directory has two major subdirectories, `TclLib` and `ImpLib`, where:

- The subdirectory `$SPHOME/TclLib` contains all the default model selections in the file `SPPROCESS.models`.
- The Tcl files are located in the subdirectories `$SPHOME/TclLib` and `$SCHOME/TclLib`.
- The subdirectory `$SCHOME/Params` contains the parameter database (see [Parameter Database on page 21](#)).
- The subdirectory `$SPHOME/ImpLib` contains all the implantation tables.

---

## File Types

The main file types used in Sentaurus Process are:

- Command file (`*.cmd`)

This is the main input file for Sentaurus Process. It contains all the process steps and can be edited. It is referred to as the *command file* or *input file*.

- Log file (`*.log` and `*.out`)

Sentaurus Process generates a `.log` file when it is run from the UNIX command line and an `.out` file when run from Sentaurus Workbench. Whichever file is written contains information about each processing step, and the models and values of physical parameters used in it. The amount of information written to the log file is controlled by the `info` argument, which is available for nearly all commands (see [Common Arguments on page 899](#)). The global default information level (0) can be changed with `pdbSet InfoDefault <n>`. Allowed values of `InfoDefault` are 0, 1, and 2 with higher values indicating more verbose output. Any value higher than 2 will be interpreted as 2.

There is a limit to the size of the log file. By default, it is `1.e9` (~1 GB). The simulation terminates if the limit is reached. This limit can be changed using the double-parameter `Log.File.Limit`:

```
pdbSet Log.File.Limit <value>
```

In addition, you can set the simulation to continue without logging any more entries after the limit is reached using:

```
pdbSet Continue.Past.Log.Limit 1
```

- Marked-up log file (`*.xml`)

When the `--xml` option is specified on the command line, Sentaurus Process generates a separate log file containing XML-like tags. This file contains exactly the same information as the `.log` file. The additional XML-like tags are used to format the `.log` file for efficient access to the information by displaying the structure of the log file content in the TCAD Logfile Browser. Tags for common modules are written automatically. You can add custom

section tags to mark important processing units with the `Section`, `SubSection.Start`, and `SubSection.End` commands. Refer to the *Utilities User Guide* for information about the TCAD Logfile Browser.

- **TDR boundary file (\*\_bnd.tdr)**

This file stores the boundaries of the structure without the bulk mesh or fields. It can be used as the structure file for the Sentaurus Mesh meshing engine and can be loaded into Sentaurus Visual for viewing. The name of a TDR boundary file can be specified using the `tdr` argument of the `init` command, and then the loaded boundary will be meshed.

- **TDR grid and doping file (\*\_fps.tdr)**

TDR files can be used to split and restart a simulation. Such restart files are saved using the `struct tdr=<c>` command because restarting requires interface data, parameter and command settings, mesh ordering information as well as bulk grid and data. If either `!pdb` or `!interfaces` is specified in the `struct` command, the TDR file will not be suitable for restarting. The TDR file can be loaded into Sentaurus Process using the `init` command, but the results of the subsequent simulation steps might differ in the simulation with the split and restart compared to a simulation of the entire flow in one attempt. TDR files store the following types of information:

- Geometry of the device and the grid.
- Distribution of doping and other datasets in the device.
- The internal structure of the mesh in Sentaurus Process required to restore the simulation mesh to the same state in memory that is present at the time of saving the file. Restart files store coordinates and field values without scaling to prevent round-off errors.
- By default, Sentaurus Process stores all changes to the parameter database made after initial loading of the database and all commands that create objects later referenced, such as refinement boxes and masks in the TDR file. A TDR file can be either reloaded into Sentaurus Process to continue the simulation or loaded into Sentaurus Visual for visualization.

The parameter settings stored in a TDR file can be viewed using `pdbBrowser -nopdb -tdr <tdrfile>` (see [Viewing Parameters Stored in TDR Files on page 36](#)).

For information about the TDR format, refer to the *Sentaurus™ Data Explorer User Guide*.

- **XGRAPH file (\*.plx)**

This file is used to save 1D distributions of the doping concentration or other fields in a specified 1D cross section. This file can be viewed by loading it into Inspect.

---

## Syntax for Creating Command Files

This section describes how to create command files manually. It is important to remember that Sentaurus Process is written as an extension of the tool command language (Tcl). This means that the full capability and features of Tcl are available in the command files as well as the interactive mode of Sentaurus Process.

Standard Tcl syntax must be followed; for example, a hash symbol (#) at the beginning of a line denotes a comment and the dollar sign (\$) is used to obtain the value of a variable. Major features of Tcl include `for` loops, `while` loops, `if then else` structures, `switch` statements, file input and output, sourcing external files, and defining procedures (functions). Variables can be numbers, strings, lists, or arrays. Refer to the literature for more information [1].

Before the command file is executed, its syntax is checked. This is accomplished by first modifying the command file so that all branches of control structures such as `if then else` and `switch` commands are executed. In addition, a special flag is set so that no structure operations or operations that depend on the structure are performed. This allows the syntax check to run quickly but thoroughly. Sometimes, the modifications made to the command file during syntax checking interfere with the definition or redefinition of Tcl variables, generating a false syntax error. In these cases, switch off syntax checking for the part of a command file using the special `CHECKOFF` and `CHECKON` commands:

```
# Skip syntax check for part of command file
# The CHECKOFF/CHECKON commands must start at the beginning of the line
# and be the only command on the line
CHECKOFF
if { $mode } {
    array set arr $list1
} else {
    set arr $list2      ;# error only if both branches are executed
}
CHECKON
# further commands are syntax checked
```

---

## Tcl Input

Sentaurus Process has been designed to optimize the use of Tcl. Some examples of this interaction include:

- Command parameter values are evaluated with Tcl. For example, `expr` can appear in the value of an expression, that is, `parameter=[expr $pp/10.0]` is valid Sentaurus Process syntax. This particular expression sets the parameter `parameter` to the value of `pp/10` if the Tcl variable `pp` was previously defined with the Tcl `set` command.

- Tcl expressions may appear in model parameter values in the parameter database. In some cases, Sentaurus Process parameters are set with Tcl commands to be a function of other parameters.
- Sentaurus Process contains many callback procedures, which can be redefined by users to provide flexibility. For example, a callback procedure is used to initialize defects after implantation.
- Many modular built-in functions are available for postprocessing, which can be combined into a Tcl script to create powerful analytic tools.
- There are special Sentaurus Process versions of `set` (`fset`) and `proc` (`fproc`), which are stored in TDR files. When simulations are restarted using a TDR file, the settings given by `fset` and `fproc` from the previous simulation will be available.

Other syntax rules to consider when writing command files are:

- One command is entered on one line only. There are two exceptions to this rule:
  - A backslash (\) is used to extend a command on to multiple lines if it appears as the last character on the line.
  - If there is an opening brace, Tcl will assume the command has not finished until the line containing the matching closing brace.
- Command parameters have the following form:
  - Boolean parameters are true if the name appears on the line. They are false if they are preceded by an exclamation mark (!).
  - Parameters that are of type *integer* or *floating point* must appear as *parameter=value* pairs.
  - String parameters are enclosed, in general, in double quotation marks (" "), for example, *parameter="string"*.
  - Lists can be enclosed in double quotation marks or braces, for example:

```
parameter= {item1 item2 ...}
parameter= "item1 item2 ..."
```

You must have a space between the equal sign and the opening brace.

**NOTE** It is important to separate the equal sign from the parameter value by a space because Tcl delimiters such as ‘’ and ‘{’ are ignored if they appear in the middle of a string. Sentaurus Process can handle *no space* between an equal sign and a double quotation mark, but it cannot correct the case where there is *no space* between an equal sign and an opening brace.

- Some parameters take a list of *keyword=value* pairs, for example:

```
epi.doping= {Boron = 1e20 Arsenic = 1e18}
```

**NOTE** For convenience, all parameters that take a numeric value will have an extra `Tcl eval` applied to them. This means that even if the value of a parameter is enclosed in braces { }, the parameter will still be evaluated. For example:

```
set val1 1.0
set val2 2.0
refinebox xrefine= {$val1 $val2}
```

will be evaluated as:

```
refinebox xrefine= {1.0 2.0}
```

---

## Specifying Materials

Materials are specified in the same way for all PDB commands that require a material parameter. For a bulk material, specify only one material. For an interface material, specify two materials combined with an underscore (\_).

Some examples of specifying materials with PDB commands are:

```
pdbSet ... Oxide ...      ;# Command applies to oxide.
pdbSet ... Oxide_Silicon ... ;# Command applies to the Si-SiO2 interface.
```

The order of materials for interfaces is lexical. However, some common material combinations have aliases. For example, `Silicon_Oxide` is an alias for `Oxide_Silicon`.

Materials are specified in the same way for all other commands that require a material parameter. For a bulk material, specify only one material. For an interface material, specify two materials: one without a slash and one with a slash (/).

Some examples of specifying materials with other commands are:

```
<command> ... oxide           ;# Command applies to oxide.
<command> ... silicon /oxide ;# Command applies to the Si-SiO2 interface.
```

The complete list of materials available can be found in the file:

```
$STROOT/tcad/$STRELEASE/lib/score-<version number>/TclLib/tcl/Mater.tcl
```

In that file, the lines that contain `mater add` create a material. For more information about creating new materials, see [mater on page 1069](#).

**NOTE** Materials present in the `Mater.tcl` file do not necessarily have parameters in the parameter database. Attention must be paid to initializing parameters for a new material.

---

## Aliases

Sentaurus Process allows more control over the names of command parameters, the abbreviations of parameter names, as well as interface names. These *aliases* only apply to parameters of built-in Sentaurus Process commands, and the `pdbSet` and `pdbGet` family of commands.

This permits clarity and uniformity to commonly used names. Another benefit is that it is easier to maintain backward compatibility for parameter names while not restricting future parameter names that could conflict with common abbreviations (that is, `V` could refer to either `vacancy` or `void`).

An explicit list of allowed aliases is maintained in the `$SCORE/TclLib` directory (see [Environment Variables on page 13](#) for information about how the location of the `TclLib` directory is determined). The `alias` command is used to view and extend the list of allowed aliases (see [alias on page 904](#)).

To print the list of aliases:

```
sprocess> alias -list
```

To view the alias of a parameter name, for example, `Vac`:

```
sprocess> alias Vac
Vacancy
```

If an alias does not exist, the same parameter name is returned:

```
sprocess> alias NotAParam
NotAParam
```

To create a new alias for a parameter name, for example, the alias `Vaca` for the parameter `Vacancy`:

```
sprocess> alias Vaca
Vaca
sprocess> alias Vaca Vacancy
sprocess> alias Vaca
Vacancy
```

For interface names, aliases for the sides can be used irrespective of the order. For example, if `Ox` is an alias for `Oxide` and `Si` is an alias for `Silicon`, then `Ox_Si` or `Si_Ox` is automatically an alias for the `Oxide_Silicon` interface. This flexibility does not apply to side-specific interface parameters. For example, `TransferRate_Si` is not automatically an alias for `TransferRate_Silicon`.

## 2: Working With the Simulator

Default Simulator Settings: SPROCESS.models File

---

# Default Simulator Settings: SPROCESS.models File

Sentaurus Process starts a simulation by reading the `SPROCESS.models` file in the `$SPHOME/TclLib` directory. This file defines various default parameters and directories used during the simulation such as:

- The path for Tcl library files
- The path for Advanced Calibration Tcl library files
- The path for implantation tables
- Default material names
- The math parameters for 1D, 2D, and 3D oxidation and diffusion simulations
- Default solution names
- Default diffusion callback procedures
- Default oxidation or silicidation reactions
- Default oxidation or silicidation solution callback procedures
- Default epitaxial growth callback procedures

The `SPROCESS.models` file is read once at the beginning of the simulation. You can override any of the default parameters after the file is read.

---

# Compatibility With Previous Releases

Occasionally, the default parameter and model settings change in Sentaurus Process to ensure that the default behavior gives robust, accurate, and computationally efficient results on current production technologies. Usually, when new models and algorithms are developed, they are optional. After some experience is gained, the default can be changed to take advantage of the new model or algorithm.

The old model and algorithm settings are collected into a file for each release and are available so that you can recover results from previous releases. Each file contains only those parameter changes that occurred for that particular release, so that if the release specified in the `Compatibility` command is older than the most recent release, the most recent release parameters are set first, followed by older releases in reverse chronological order (see [Compatibility on page 915](#)).

For example, the command `Compatibility K-2015.06` issued for Version N-2017.09 will first apply parameters consistent with M-2016.12, then with parameters consistent with L-2016.03, and finally parameters consistent with K-2015.06. Aliases are available for the

release name so you do not need to know the release foundation letter. For example, 2015.06 can be used instead of K-2015.06.

Files with the compatibility parameter settings are stored in \$STROOT/tcad/\$STRELEASE/lib/sprocess/TclLib/Compatibility. These files provide a useful list of all default parameter changes for each release.

**NOTE** As a result of code corrections and numeric accuracy limitations, exact reproduction of results from previous releases is not always possible.

**NOTE** If the Compatibility command is used, it must be the first command in a command file so that all subsequent commands that depend on the defaults take into account the compatibility setting.

For example, to apply the defaults of Version M-2016.12, the first line of the command file must be:

```
Compatibility 2016.12
```

**NOTE** The Compatibility command does not change the default parameter and algorithm settings for Sentaurus Mesh, Sentaurus Structure Editor, and the MGOALS module. To change the backward compatibility setting for MGOALS, see [MGOALS Backward Compatibility on page 823](#).

---

## Parameter Database

The parameter database stores all Sentaurus Process material and model parameters as well as global information needed for save and reload capabilities. There is a hierarchical tree directory inside the Params directory, which stores the default values. (To locate the Params directory, see [Environment Variables on page 13](#).)

Data is retrieved using the pdbGet command and is set using the pdbSet command. The pdbGet and pdbSet commands are checked for correctness of syntax, and they print the allowed parameter names if a mistake is made. These commands are used to obtain and set all types of data stored in the parameter database: Boolean, string, double, double array, and switch.

The higher-level pdbSet and pdbGet commands call lower-level type-specific commands (`pdbGetBoolean`, `pdbGetDouble`, `pdbGetDoubleArray`, `pdbGetString`, `pdbGetSwitch`, `pdbGetSwitchString`, `pdbSetBoolean`, `pdbSetDouble`, `pdbSetDoubleArray`, `pdbSetString`, and `pdbSetSwitch`) that are not checked for errors

## 2: Working With the Simulator

### Parameter Database

and, therefore, are not recommended for typical use. These commands have a slight performance advantage and are used internally.

You can set some parameters in a region-specific manner. Regions can be named with the region and deposit commands and, if region-specific parameters exist, they will override the material-specific parameters if any. However, there are many circumstances where this will not give the desired behavior. In that case, you must create a new material that inherits its parameters from an existing material. Then, you must change the material properties of the new material as needed (see [Like Materials: Material Parameter Inheritance on page 24](#)).

Inside the `Params` directory are subdirectories that define the highest level nodes in the database. Inside each subdirectory is a file `Info`, which contains parameters of that level. In addition, directories in the database have named files that contain parameters, which are under the node defined by the file name. For example, in the `Params` database, there is a directory called `Silicon`, which contains a file `Info`. The parameters inside `Info` are located under the `Silicon` node. As another example, inside the `Silicon` directory is another file `Interstitial` that contains parameters under the `Interstitial` node, which is under the `Silicon` node.

Inside the files of the parameter database are commands that set the database parameters. The commands have the form:

```
array set $Base { <NAME> { <TYPE> <VALUE> } }
```

where:

- `<NAME>` is the parameter name.
- `<TYPE>` is one of `Boolean`, `String`, `Double`, `DoubleArray`, or `Switch`.
- `<VALUE>` is a Tcl expression that sets the default value.

It is often necessary to enclose the `<VALUE>` expression in braces. Some Tcl procedures have been created to increase the usefulness of `<VALUE>` expressions. For example, in many places in the database, the built-in function `Arrhenius` is used to set the value of a parameter. Parameters that contain a Tcl function are evaluated at each diffusion time step so that temperature-dependent parameters will update correctly during a temperature ramp. It is important to remember that the `Arrhenius` function uses the global Tcl variable for temperature, which defaults to room temperature.

If you start Sentaurus Process and call the `pdbGet` command of a parameter that contains an `Arrhenius` function, it will return the value of that parameter at room temperature. The temperature can be changed with the `SetTemp` function. Subsequent calls to the `Arrhenius` command through `pdbGet` return values based on the given temperature. In addition, the `diffusion` command changes the global temperature for each time step, and the temperature after diffusion will be same as the temperature in the last diffusion time step.

Other functions that appear in the pdb parameters are `DiffLimit`, which calculates a diffusion-limited reaction rate given the diffusivity of the two reacting species, and `pdbGet*` functions, which allow parameters to be set as a function of other parameters.

For the `DoubleArray` type, a Tcl list is set that is ordered pairwise:

`{key1 value1 key2 value2 ...}` where the parameter setting for `key1` is `value1`.

Material parameters can be stored under the known region name. To set and obtain the parameter value, use the region name instead of the material name. If the parameter is not found under the region name, it is taken from the material of that region.

Sentaurus Process writes directly to the parameter database in a number of ways. Mostly this is performed to save information for reload capabilities using the TDR format. Data written by the program into the parameter database is not available within the default `Params` directory or the Parameter Database Browser, but can be read using the `pdbGet` command.

For information about the TDR format, refer to the *Sentaurus™ Data Explorer User Guide*.

---

## Parameter Inheritance

The parameter database has a parameter inheritance feature where parameters at a certain level or node can inherit the parameters from another node at the same level. The inherited parameters can be overwritten with new values. Inheritance is indicated by the presence of a special parameter named `Like`. In one of the parameter database files, the `Like` parameter is specified as follows:

```
array set $Base {Like <Node>}
```

which means that parameters at the level of the file inherit parameters from `<Node>`, which should be another node at the same level. For example, the file:

```
Params/Silicon/Arsenic/Info
```

contains the line `array set $Base {Like Dopant}`, which indicates that `Arsenic` in `Silicon` should inherit the common parameters of all `Dopant` species in `Silicon`. Other parameters specified in that file indicate parameter settings specific to `Arsenic` in `Silicon`.

It is also possible to use inheritance to create new parameters from the command line using the `pdbLike` command (see [pdbLike on page 1103](#)). For example, assuming `MyBoron` is defined as the solution:

```
pdbLike Silicon MyBoron Boron
```

## 2: Working With the Simulator

### Parameter Database

then, MyBoron will inherit Boron parameters including user-defined and callback parameters for MyBoron in silicon. The new parameters are used to set up diffusion equations for MyBoron.

---

## Like Materials: Material Parameter Inheritance

The parameters of a material can be inherited from the parameters of another material using the special `Like` parameter in the PDB. When this is the case, the two materials are referred to as *like materials*. This can be used to specify different settings in different regions. First, a new material is created and made to be *like* an existing material using:

```
mater add name=<c> new.like=<c>
```

where:

- `name` specifies the name of the material to be created.
- `new.like` is the name of the existing material from which all default values are inherited.

**NOTE** It is important to use the `mater` command instead of directly creating the `Like` parameter because the `mater` command will make all interfaces to the new material like the appropriate interface to the existing material.

**NOTE** Reaction specifications, such as oxidation, silicidation, and epitaxy, are not stored in the PDB. Therefore, for a new material to react, a new reaction command must be issued (see [reaction on page 1146](#)).

---

## Interpolation Between Like Materials

By default, data is interpolated between *like* materials, for example, when you insert a region that overlaps an existing region of a like material. The inheritance direction does not matter; either the inserted material is like the existing material, or the existing material is like the inserted material.

To prevent interpolation between a material and other materials that are like it, use:

```
mater name=<c> add !like.interpolate
```

## Interface Parameters

When using the Parameter Database commands and the Alagator language, interfaces are specified as a pair of materials separated by an underscore (\_), for example, `Gas_Oxide` and `Oxide_Silicon`. The official name follows alphabetic order, and the first letter is capitalized. However, aliases are provided that allow their order to be reversed; some shorter names are allowed; and all lowercase is generally available.

As an example of setting an interface parameter, the following command sets the numeric tolerance `Abs.Error` at the gas–silicon interface to `1e3`:

```
pdbSet Gas_Silicon Vac Abs.Error 1e3
```

---

## Alloy Materials and Parameter Interpolation

Material parameters in random alloys are typically assumed to depend on the mole fraction. To capture this effect, Sentaurus Process uses automatic mole fraction–dependent parameter interpolation. After a material has been set up as an alloy of a set of base materials, the mole fraction is updated automatically if the base material fields are modified, for example, during implantation or diffusion. All material parameters that have been interpolation *enabled* will automatically vary throughout regions of the alloy material depending on the local mole fraction of the base materials. For example, the alloy  $\text{Si}_{(1-x)}\text{Ge}_x$ , which is given the name `SiliconGermanium` (and the shorthand alias `SiGe`) in Sentaurus Process, is composed of the base materials `Silicon` and `Germanium`. The base material concentration and the mole fraction ‘ $x$ ’ (`xMoleFraction`) are stored as fields in the material `SiliconGermanium`.

### Using Parameter Interpolation

Switches are available to turn parameter interpolation on and off at different levels: global, module, material, region, and parameter. By default, parameter interpolation is used in any material that is specified as an alloy (see [Defining Alloy Materials on page 28](#)).

The default list of alloy materials includes `SiliconGermanium`, `AlGaAs`, `AlInGaAs`, `InGaAs`, `InGaAsP`, `GaAlN`, `GaAsP`. For backward-compatibility reasons, interpolation is not used in `Silicon` and `Germanium` by default.

To switch on interpolation for `Silicon` with a `Germanium` field (of significant mole fraction), use:

```
pdbSet Silicon Skip.Parameter.Interpolation 0
```

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### Parameter Database

## Interpolation Function Types

Besides the default linear interpolation, the available interpolation functions are parabolic, piecewise linear table, logarithmic, and user defined.

Not all interpolation types are available for all parameters. Further details regarding available interpolation types for specific parameters and other alloy-specific information can be found in the following sections:

- [Monte Carlo Implantation Into Alloy Materials on page 132](#)
- [Low-to-High Germanium-Doped SiGe Model on page 243](#)
- [Diffusion in III–V Compounds on page 251](#)
- [Parameter Interpolation in Alloys on page 426](#)
- [SiGe and Mole Fraction–Dependent Growth on page 586](#)

In addition, to see which parameters have been handled by the mole fraction–dependent interpolation, you can use the `print_interpolated_params` command (see [print\\_interpolated\\_params on page 1136](#)).

The following commands can be used to choose one of the nonlinear interpolation methods.

This command is only for logarithmic interpolation:

```
pdbSet <Alloy Material> Log.Interpolated.Params {<list of parameters>}
```

For all other types:

```
pdbSet <parameter name>.<interpolation type> {<interpolation coefficients>}
```

Many of the interpolation types require coefficients. For these, it is necessary to set the coefficients using the composite name `<parameter>.<interpolation type>`.

Table 3 Nonlinear mole fraction–dependent interpolation types

Interpolation	<interpolation type>	Coefficients
Linear	(default)	(Default - no coefficient)
Parabolic	X2	Second-order coefficient.
Piecewise linear	XTable	Table of mole fraction–value pairs.
User defined	Function	Only available for diffusion parameters. Specify a script that returns an Alagator expression of <code>xMoleFraction</code> (and <code>yMoleFraction</code> and <code>zMoleFraction</code> ).
Logarithmic	Use parameter <code>Log.Interpolated.Params</code>	(No coefficients)

For example, to use parabolic interpolation for the BulkModulus in SiGe, specify:

```
pdbSet SiliconGermanium Mechanics BulkModulus.X2 5e10
```

The parameters are interpolated with the parameter values of silicon and germanium materials when the following conditions are satisfied:

- The parameter values for SiGe material are not set by users.

When you set the value for a parameter for SiGe material, it is assumed that you want to use this value instead of the interpolated value. For example, when using the command:

```
pdbSet SiGe Boron Dstar 1E-10
```

Dstar is not interpolated. Instead, the 1E-10 value is used. Note that the parameter is not interpolated even when you set it to the same value as the default value.

- The parameters are not in the list of `Not.Interpolated.Params` in SiGe material.

## Linear Interpolation

For the parameter of a ternary material,  $A_{(x)}B_{(1-x)}C$ :

$$P_{A_{(x)}B_{(1-x)}C} = P_{AC} \cdot x + P_{BC} \cdot (1 - x) \quad (1)$$

For the parameter of a quaternary  $A_{(x)}B_{(y)}C_{(1-x-y)}D$ :

$$P_{A_{(x)}B_{(y)}C_{(1-x-y)}D} = P_{AD} \cdot x + P_{BD} \cdot y + P_{CD} \cdot (1 - x - y) \quad (2)$$

For the parameter of a quaternary  $A_{(x)}B_{(1-x)}C_{(y)}D_{(1-y)}$ :

$$P_{A_{(x)}B_{(1-x)}C_{(y)}D_{(1-y)}} = P_{AC} \cdot xy + P_{AD} \cdot x(1 - y) + P_{BC} \cdot (1 - x)y + P_{BD} \cdot (1 - x)(1 - y) \quad (3)$$

## Parabolic Interpolation

The extension x2 of a parameter defines a parabolic dependency on the x–mole fraction of a ternary compound. The parabolic interpolation is performed by:

$$P_{A_{(x)}B_{(1-x)}C} = P_{AC} \cdot x + P_{BC} \cdot (1 - x) + P.X2_{ABC} \cdot x \cdot (1 - x) \quad (4)$$

For example, when the energy bandgap at 300 K ( $E_{g300}$ ) for InGaAs shows parabolic dependency on the x–mole fraction as follows:

$$E_{g300}(\text{InGaAs}) = E_{g300}(\text{GaAs}) \cdot x + E_{g300}(\text{InGa})(1 - x) - 0.485 \times (1 - x) \quad (5)$$

the following command is needed:

```
pdbSetDouble InGaAs Potential Eg300.X2 -0.485
```

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#### Logarithmic Interpolation

Some parameters such as diffusivity are more physically appropriate to be logarithmically interpolated despite that the simulation may require more time than linear interpolation due to its complexity. The parameter value in logarithmic interpolation is taken from its logarithmic value. For example, Eq. 4 is applied by:

$$P_{A(x)B(1-x)C} = \exp(\ln(P_{AC})x + \ln(P_{BC})(1-x) + \ln(P.X2_{ABC})x \cdot (1-x)) \quad (6)$$

The parameter list for logarithmic interpolation is specified by:

```
pdbSetString <alloy> <p_1> ... <p_n> Log.Interpolated.Params {<param_list>}
```

For example:

```
pdbSetString InGaAs Silicon IntIII Log.Interpolated.Params { D Dpair }
```

#### User-Defined Interpolation

For parameters that cannot be interpolated with the abovementioned functions, you can define your own interpolation function with the Tcl proc command. The function can be defined using the .Function extension, that is, <param>.Function.

The Tcl proc command must return the string expression depending on mole fractions. The following is an example for the energy bandgap of SiGe since the mole fraction dependency shows abrupt change due to the transition between the X-valley and the L-valley:

```
pdbSet SiGe Potential Eg300 "[pdbGet Si Potential Eg300]"
pdbSet SiGe Potential delEg.Function {[mySiGeDelEg]}
fproc mySiGeDelEg {} {
    set delEgX "(-0.3758*((0.7795-xMoleFraction)^2)+0.2315)"
    set delEgL "0.2406*exp(-((xMoleFraction-1)/0.1176)^2))"
    return "(-$delEgX - $delEgL)"
}
```

#### Interpolation at Interfaces

At a material interface, parameters are interpolated with the parameter values of the neighbor material with Si and one with Ge. For example, the parameter values of an interface with oxide are interpolated with the parameter values of Oxide\_Silicon and Germanium\_Oxide.

#### Defining Alloy Materials

An alloy material has the parameter MoleFractionAtoms of the Parameter Database that specifies the mole fraction definition. The MoleFractionAtoms parameter is set internally by reading the Molefraction.txt file in the \$STROOT/tcad/\$STRELEASE/lib directory,

which is shared with Sentaurus Device. This guarantees identical definitions for both tools. The parameters of an alloy that depends on mole fractions are interpolated with the parameter values of the base materials.

The parameter `Derived.Materials` of the Parameter Database is used to define a non-alloy material to be handled like an alloy material. For example, the Ge-doped silicon region where the maximum Ge concentration exceeds  $1 \times 10^{21} \text{ cm}^{-3}$  can be handled like SiGe by the following commands:

```
pdbSet Si Derived.Materials {SiGe}  
pdbSet SiGe Ge Min.Conv.Conc 1E21
```

---

## Regionwise Parameters and Region Name-Handling

Many parameters in the parameter database can be specified regionwise including parameters related to meshing, parameters for both analytic implantation and Monte Carlo implantation, and mechanics parameters. Those parameters used by Alagator as part of equations and terms, however, cannot be specified regionwise: this includes all dopant diffusion parameters and all oxidation and silicidation parameters. For the rest of the parameters, internally, the program checks if there is a regionwise specification of the parameter; if not, the materialwise specification is used.

The name of regions can be specified with the `region` command and `deposit` command; however, the name:

- Must not contain an underscore (`_`) or a period (`.`) because these characters have special meaning.
- Must be different than an existing material name.

During the course of the simulation, geometric operations such as etch and reflect can split regions in two. If this happens, the history of the region is maintained through its name. For example, if a region is originally named `layer1` and it is etched into two pieces, they will be named `layer1.1` and `layer1.2` according to rules given below.

These two regions will inherit the parameters of `layer1`. Furthermore, parameters for `layer1.1` and `layer1.2` also can be specified separately. If a subsequent step such as a deposit reunites `layer1.1` and `layer1.2`, the region will be given the name `layer1`. Conversely, if `layer1.1` is split into two regions, the regions will be named `layer1.1.1` and `layer1.1.2`, and so on. In this way, regionwise parameter specification is preserved for the life of the region or its parts.

The numbering of split regions is performed according to the spatial location of the pieces. The lowest point of each piece to be renamed is found (in the coordinate system of Sentaurus Process, this would be the largest x-coordinate). To avoid numeric noise, the coordinates are

## 2: Working With the Simulator

### Parameter Database

compared with a specified epsilon given by `pdbGet Grid RenameDelta` (hereafter, referred to as `RN`). If the x-coordinates of the pieces to be renamed are not within `RN` of each other, the regions are ordered from lowest to highest, that is, from the highest x-coordinate to the lowest. If any piece has its lowest coordinate within `RN`, its y-coordinate is compared, that is, from the lowest coordinate to the highest.

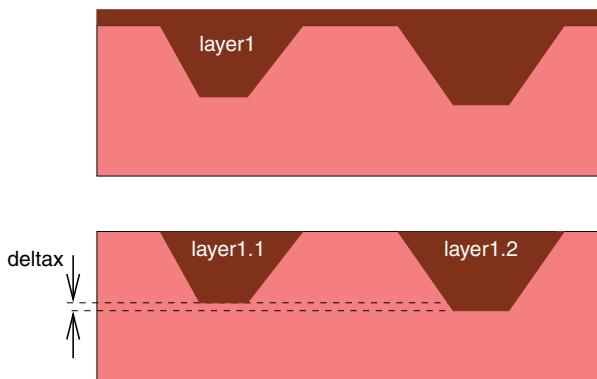


Figure 3 Illustration of region-naming rules

For example, in [Figure 3](#), `layer1` is split into two regions and the quantity `deltax` is less than `RN`, so the region on the left is given the name `layer1.1` and the region on the right is given the name `layer1.2`. If `deltax` had been greater than `RN`, the region on the right would have been given the name `layer1.1` because it would have been considered lower than the region on the left. Similarly, in three dimensions, first x and y are compared, and if they are both within `RN`, z is used for ordering, that is, from the lowest coordinate to the highest.

You can apply the above operation to the whole structure with `grid rename`. In this case, all the regions are renamed similarly to the above rules but, instead of the root being chosen by the user, all regions of the same material have the root given by the names of the materials and the extension is `_<n>` where `<n>` is the region number, for example `Silicon_1`, `Silicon_2`, and so on. This should only be used as a postprocessing step because all region-specific parameters no longer apply when the name of a region has changed.

For example, if two oxide layers are grown, one with steam (if it is the first oxide region, its name would be `Oxide_1`) and one from pure O<sub>2</sub> (which would be `Oxide_2` if it were the second oxide region), they can have different densities. This can be considered in an MC implantation using:

```
pdbSetDouble Oxide_1 MassDensity <wet oxide density>
pdbSetDouble Oxide_2 MassDensity <dry oxide density>
```

where `<wet oxide density>` and `<dry oxide density>` would be replaced with values given in g/cm<sup>3</sup>.

Sentaurus Process automatically unites regions with the same material type. For example, if silicon is deposited on top of an existing silicon region, both regions are united, so there will be only one silicon region. If regions must be united and region names do not follow the rules mentioned in this section, the united region will take the name of one of the materials in the united region.

---

## Parameter Database Browser: Viewing the Defaults

The Parameter Database (PDB) Browser is a graphical representation of the parameter database that allows you to view and edit parameters. The PDB Browser has three distinct areas (see [Figure 4 on page 32](#)):

- Parameter hierarchy overview in a tree structure representation.
- Parameter information in a spreadsheet representation. The columns are Parameter, Type, Value, Unit, Evaluate, Comment, Tool, and Info Level (hidden by default).
- Graphic window to plot the parameter dependency on the temperature.

The status bar has three indicators that show:

- The temperature used in temperature-dependent functions such as Arrhenius.
- The temperature point set for the x-axis.
- The x-coordinate and y-coordinate of the pointer in the graphic window.

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### Parameter Database Browser: Viewing the Defaults

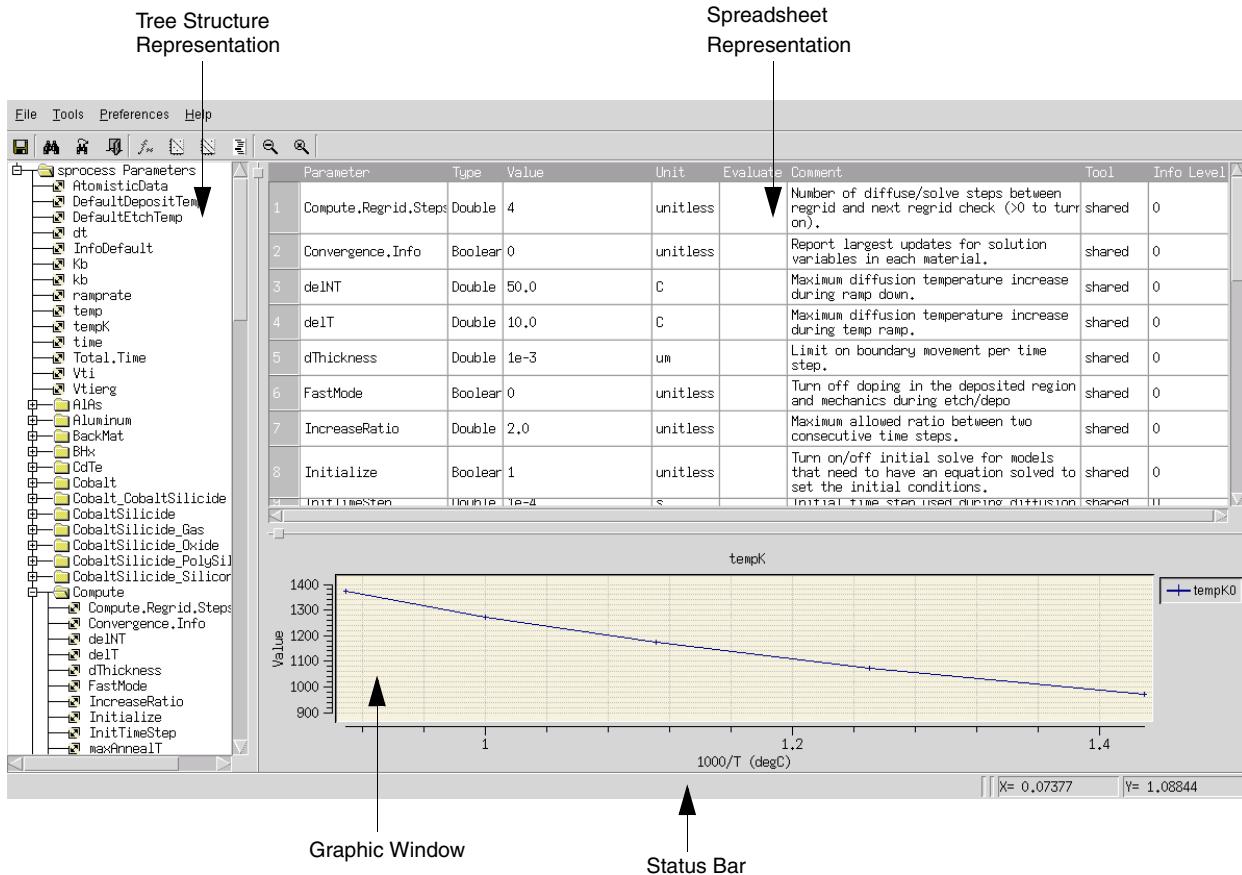


Figure 4 Parameter Database Browser

## Starting the Parameter Database Browser

To start the PDB Browser from the command line, type:

```
pdbBrowser
```

This searches for the parameter database in the same location as Sentaurus Process.

You can set the environment variables SPHOME and SCHOME to change the location of the parameter database for the PDB Browser and Sentaurus Process (see [Environment Variables on page 13](#)).

You can select **Tools > Filter** to choose which parameters to display.

To view parameters in a command file merged with defaults, use:

```
sprocess --pdb <command file>
```

To view only the parameters specified as input in a command file, use:

```
sprocess --ponly <command file>
```

---

## PDB Browser Functions

The following functions are available from the **File** and **Tools** menus:

### File > Export Node

Saves the selected node into a specified file in tab-delimited format.

### File > Export Tree

Saves the entire parameter database into a specified file in tab-delimited format. The fields of the file are **Parameter Name**, **Type**, **Value Evaluation**, **Original Value**, and **Comments**.

### Tools > Evaluate

Evaluates the value of the selected parameter and displays the result in the Evaluate column of the spreadsheet. Values can contain Tcl expressions.

### Tools > Plot

(Applies only to parameters of type *double* and *double array*.) Plots the dependency of the selected parameter on the temperature in logarithmic coordinates versus 1/T. The default set of temperature values is { 700.0 800.0 900.0 1000.0 1100.0 }. The resulting graphs are displayed in the graphic window; otherwise, an error message is displayed.

### Tools > Plot Over

The same as **Plot** but it does not clear the graphic window of previous graphs.

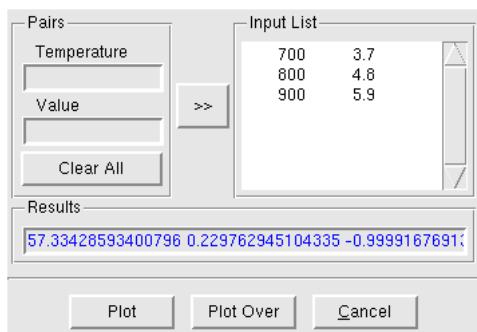
**NOTE** You can zoom in by dragging the mouse. To zoom out, use the middle mouse button, or click the **Zoom Out** and **Zoom Off** buttons.

## 2: Working With the Simulator

### Parameter Database Browser: Viewing the Defaults

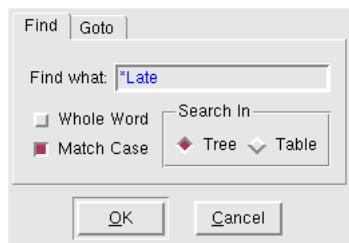
#### Tools > Arrhenius Fit

Using the Arrhenius Fit dialog box, you can find the best prefactor and energy for an Arrhenius fit of a given profile, taken from the list of temperature–value pairs. The results can be plotted in the graphic window:



#### Tools > Find, Tools > Find Next

Matches the pattern entered against parameter names according to the options selected in the Find dialog box. Patterns can include regular Tcl expressions. The match is highlighted when found:



#### Tools > Goto Line

Highlights a table row or tree node that corresponds to the number entered.

#### Tools > Filter

Selects which parameters to display.

#### Tools > Info Level

Chooses which parameters to display ranging from basic parameters to all parameters.

### Viewing Parameter Information

Double-clicking a nonempty cell in the spreadsheet allows you to view the corresponding parameter information in a separate window. To close the window, click the **Close** button.

**NOTE** To display a shortcut menu, right-click a parameter and select commands for editing, evaluating, or plotting.

---

## PDB Browser Preferences

The PDB Browser allows you to reset the default settings for the following values using the **Preferences** menu, the shortcut keys, or the shortcut menu of the graphic window:

### Preferences > Editor > Change Editor

Resets the default editor.

### Preferences > Editor > Reset Update Time

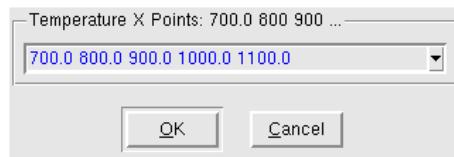
Resets the update interval.

### Preferences > Graph > Set Temperature

Sets the global temperature used in the temperature-dependent functions. Default: 1000.0.

### Preferences > Graph > Reset X Points

Displays the Reset Temperature Points dialog box where you set the x-axis temperature points. The default set is {700.0 800.0 900.0 1000.0 1100.0}:



### Preferences > Graph > Data Point Symbol

Sets the symbol to use for data points.

### Preferences > Graph > X Scale

Resets the x-scale to logarithmic or linear.

### Preferences > Graph > Y Scale

Resets the y-scale to logarithmic or linear.

### Preferences > Tree Node

Hides the node tip or shows the node tip.

## **2: Working With the Simulator**

Parameter Database Browser: Viewing the Defaults

### **Preferences > Info Level**

Shows or hides the Info Level column of the spreadsheet.

### **Preferences > Font > Family**

Changes the font family.

### **Preferences > Font > Size**

Changes the font size.

### **Preferences > Cursor**

Changes the style of the cursor.

---

## **Viewing Parameters Stored in TDR Files**

Parameters stored in TDR files can be viewed using the `pdbBrowser` command run from the command line instead of through Sentaurus Process. By default, the PDB Browser reads parameters from the Sentaurus Process database directory (which can be changed with the `SPHOME` and `SCHOME` environment variables). In addition, parameters stored in a TDR file can be read in using the `-tdr <filename>` option of the PDB Browser. Parameters that appear in the parameter database are overwritten by those contained in the TDR file, so the resultant parameter set will be the same as if Sentaurus Process had read in the file. On the other hand, it is also useful to know which parameters are only in the TDR file. To read only those parameters, the database reading can be switched off using the `-nopdb` command-line option.

For example, the following command reads the PDB Browser and then reads the parameters from the `n10_fps.tdr` file, overwriting values contained in the parameter database:

```
> pdbBrowser -tdr n10_fps.tdr
```

For example, the following command reads only the parameters in the `n10_fps.tdr` file:

```
> pdbBrowser -nopdb -tdr n10_fps.tdr
```

## Understanding Coordinate Systems

Sentaurus Process and related tools use different coordinate systems.

### Wafer Coordinate System

The wafer coordinate system is fixed with respect to the wafer flat or notch, and is used to define the relationship of all other coordinate systems to the physical wafer.

The wafer x- and y-axes form a naturally oriented coordinate system when the wafer is drawn with the flat pointing down as shown in [Figure 5](#). This coordinate system is used for layout information, such as mask locations, and for setting a cutline using the `CutLine2D` command.

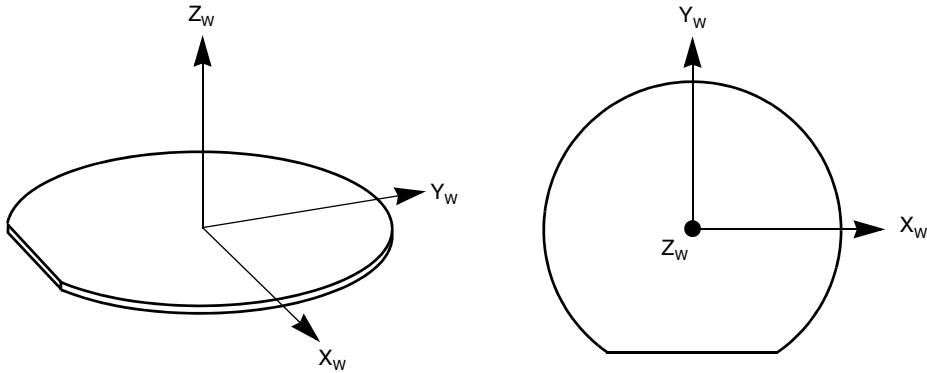


Figure 5 Wafer coordinate system

### Simulation Coordinate System

The simulation coordinate system is used to define the mesh for the simulation. The default coordinate system is the *unified coordinate system* (UCS).

The visualization coordinate system is the UCS as well.

## 2: Working With the Simulator

### Understanding Coordinate Systems

In the UCS, the x-axis points into the wafer and the y-axis is rotated with respect to the wafer y-axis. [Figure 6](#) shows the UCS. Simulations in one dimension use only the x-axis. Simulations in two dimensions use only the x- and y-axes.

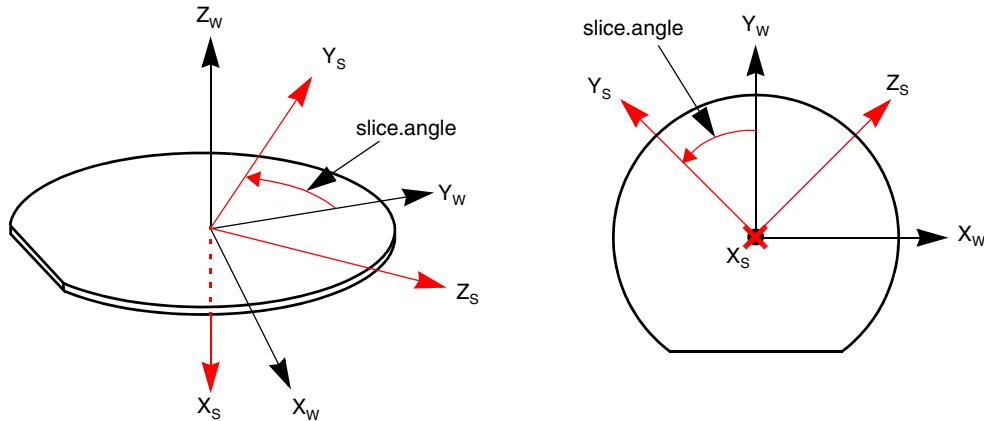


Figure 6 Unified coordinate system (`slice.angle= 45`)

The rotation of the simulation axes with respect to the wafer axes is given by the `slice.angle` parameter of the `init` command. The slice angle is measured from the wafer y-axis to the simulation y-axis with positive angles counterclockwise about the wafer z-axis.

The default value of `slice.angle` is  $-90^\circ$ . This causes the simulation y-axis to match the wafer x-axis, which is the usual cut direction through the layout for 2D simulations (see [Figure 7](#)).

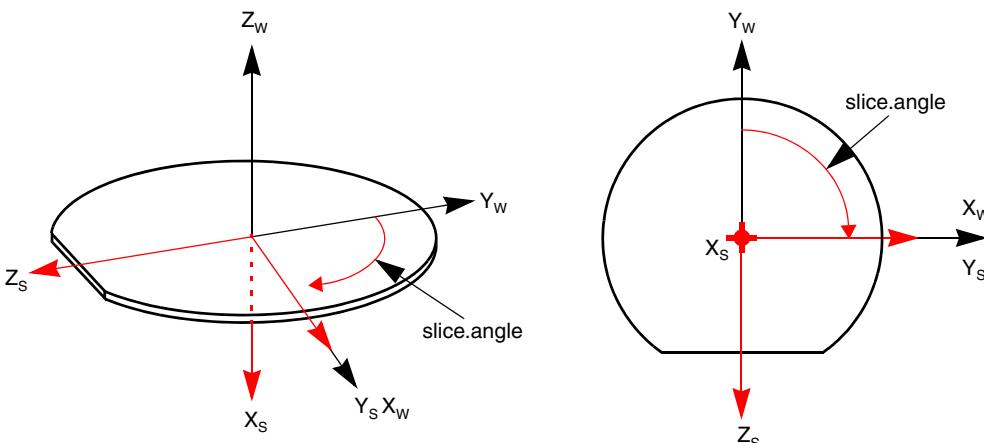


Figure 7 Unified coordinate system when using default value of `slice.angle` ( $-90^\circ$ )

**NOTE** For backward compatibility, the DF-ISE coordinate system is still available, but it is not recommended.

---

## Creating and Loading Structures and Data

The first step in most simulations is either to load an existing structure or to create a new one. New structures are created through a combination of the `line`, `region`, and `init` commands. The initial mesh is a tensor-product mesh where the density of lines is specified using the `line` command, and the regions are defined by specifying tags in the `line` commands and defined in the `region` command. The initial regions are always defined as axis-aligned rectangles in two dimensions and axis-aligned bricks in three dimensions.

---

### Defining the Structure: The `line` and `region` Commands

The `line` and `region` commands are used together to define the structure. In the `init` command, the structure is actually formed. Care must be taken when creating a structure because there are few checks for errors.

These rules must be followed to obtain a valid structure:

- If this is not the first structure being created in a command file, the command `line clear` must be issued to remove `line` commands and stored mesh ticks.
- Line locations must be given in increasing order.
- The region boundaries are defined by tagged lines. Tagged lines are created with the `line` command where the parameter `tag` has been set (as well as the `location` parameter).
- At least one `region` command must be given to define the substrate.
- Regions must have a material specification, except for the `substrate` case described below.
- Regions must have the same dimensionality as the `line` commands used (that is, if `line y` is given, a 2D region is expected with `ylo` and `yhi` set in the `region` command).
- The `spacing` parameter of the `line` command is used to create lines between user-defined lines, so that not every line must be specified in the command file. Sentaurus Process smoothly grades the line density between user-defined lines to match as closely as possible the spacing at each user-defined line. In addition, there will be lines at locations given by the `location` parameter of the `line` command. By default, the `spacing` parameter is extremely large, so that if it is not set, only lines given by the `location` parameter will be in the mesh.
- The `*lo` parameter refers to the lowest coordinate value, that is, the location of the line corresponding to the `xlo` tag must be less than the coordinate corresponding to the `xhi` tag.
- The `region` command can be used to tag a region as a substrate in two ways:
  - If the region is being defined with the material name and the parameters `*hi` and `*lo`, the Boolean keyword `substrate` will tag this region as the substrate.

- If the structure is being loaded from a previously saved file, the command:

```
region name=<c> substrate
```

will tag the region with <c> as the name of the substrate. This is the only occasion when the `region` command will be called *after* the `init` command.

Considerations when creating structures are:

- For 2D and 3D simulations, it is advantageous to create a coarse mesh in the lateral (that is, y- or z-directions) because lines created with the `line` command run all the way through the structure. Often, finer spacing in the y- or z-direction is required near the surface; whereas, further in the bulk, a coarser spacing is required (to minimize the size of the problem).
- When MGOALS is used for etching and deposition, it automatically creates a local refinement near interfaces that does not run the length of the structure.
- To specify refinement boxes, use the `refinebox` command.

---

## Creating the Structure and Initializing Data

The `init` command is used to create the structure. If the `line` and `region` commands have been given to create a structure from the beginning, the `init` command does not require any options. It will take the structure definition and create a new structure.

Many process steps such as etching and deposition require a gas mesh. By default, Sentaurus Process does not add a gas mesh during the `init` command, but delays creating the gas mesh until it is needed. To add the gas mesh immediately, use the command:

```
pdbSet Grid AddGasMesh 1
```

**NOTE** The parameter must be set before the `init` command to generate the gas mesh during the `init` command.

There are different ways to initialize fields at the time the initial structure is created from `line` and `region` commands:

- To initialize data everywhere in the structure, a field specification can be given in the `init` command.
- To initialize data in one particular region only, a field specification is given in the `region` command.

In both the `init` and `region` commands, the `field` parameter specifies the name of the data field that will be created, and either the `concentration` parameter or the `resistivity` parameter is used to specify the value created. Although initialization was intended for dopants, a field with any name can be initialized with the `concentration` parameter.

However, because the `init` command will only create a field with nodal values and, because stresses are computed on elements, the `init` command must not be used to initialize stress values (use instead either the `stressdata` command or the `select` command). The `resistivity` parameter only works for fields that have the resistivity parameters set (which by default are only As, B, P, Sb, and In in silicon).

The `init` command also can read a structure from a file, for example:

```
init tdr= file      ;# Read geometry, data, and PDB parameters from file.tdr
```

The TDR format is the default format and can store all the information necessary to restart a simulation when using ‘splits’ in Sentaurus Workbench. This format stores all `pdb` parameter settings as well as numerous other settings coming from commands (see [Saving a Structure for Restarting Simulations on page 45](#)).

The `init` command specifies the principal wafer orientation (`wafer.orient`), the lateral crystal orientation of the wafer flat or notch (`notch.direction`), and the `slice.angle` of the `implant` command, that is `angle`:

```
init wafer.orient= {<i> <j> <k>} notch.direction= {<i> <j> <k>}  
slice.angle=<n>
```

where the first set of `<i>`, `<j>`, and `<k>` specifies the crystallographic (Miller) indices for the wafer orientation *plane*, and the second set of `<i>`, `<j>`, and `<k>` specifies the Miller indices for the *direction* of the wafer notch or the primary flat orientation, which is a direction pointing from the center of the wafer to the flat. For more information about the wafer orientation and the slice angle, see [2D Coordinate System on page 61](#).

You also can set the `slice.angle` using a 2D cutline, for example:

```
init slice.angle= [CutLine2D <x1> <y1> <x2> <y2>]
```

The first two values define the start point, and the third and fourth values define the endpoint in the wafer plane. The two points are defined in the wafer coordinate system (see [Wafer Coordinate System on page 37](#)).

---

## Defining the Crystal Orientation

Generally, the orientation of a hexagonal crystal system can be described using four Miller indices `<ijtk>`; whereas, only three Miller indices `<ijk>` are needed for other systems. In a hexagonal crystal system, the sum of the first three indices equals zero ( $i+j+t = 0$ ); therefore, the third index `t` is redundant and can be omitted. For simplicity and consistency, the wafer orientation and the flat orientation are specified using three Miller indices for all lattice systems including hexagonal.

The crystal orientation of the wafer is established by specifying the Miller indices of the wafer surface and the wafer flat. The `wafer.orient` and `notch.direction` (originally `flat.orient`) arguments of the `init` command specify the Miller indices of the wafer z-axis and negative y-axis, respectively. The wafer surface orientation (whose surface normal is chosen as the wafer z-axis) is set using `wafer.orient= {<i> <j> <k>}` where `<i>`, `<j>`, and `<k>` are the crystallographic (Miller) indices of the plane. The notch direction or the flat orientation (a direction that coincides with the wafer negative y-axis) can be set arbitrarily, but it must be orthogonal to the surface normal of the wafer orientation.

The default surface orientation is 100 and the default flat orientation is a 110 direction for all lattice systems.

**NOTE** The `wafer.orient` and `notch.direction` arguments of the `init` command apply to any crystalline systems in the structure. However, these settings are superseded by the material-specific wafer orientation (`vertical.orient`) and flat orientation (`horizontal.orient`) as specified in the `mater` command.

[Table 4](#) lists the crystallographic directions of the wafer axes for the most common crystallographic orientations of the wafer as shown in [Figure 5 on page 37](#).

Table 4 Miller indices of wafer axes for each value of `wafer.orient`  
(wafer axes are defined in [Figure 5](#))

Wafer orientation	X <sub>w</sub>	Y <sub>w</sub>	Z <sub>w</sub>
100	[1̄10]	[110]	[001]
110	[001]	[1̄10]	[110]
111	[1̄1̄2]	[1̄10]	[111]

To facilitate simulations of hybrid orientation technology, Sentaurus Process predefines three materials (`Silicon`, `Silicon110`, and `Silicon111`) for crystalline silicon. These materials have exactly the same properties, except for the default crystal orientations that are `<100>`, `<110>`, and `<111>` for `Silicon`, `Silicon110`, and `Silicon111`, respectively.

---

## Automatic Dimension Control

The maximum dimension of a simulation is determined by the specified `line` commands:

- `line x` commands define the extensions in the vertical direction and are required for 1D, 2D, and 3D simulations.
- If, in addition, `line y` commands are specified, the maximum dimension of the simulation will be at least two dimensions.

- If, in addition, `line z` commands are specified, the maximum dimension of the simulation will be three dimensions.

By default, Sentaurus Process delays the creation of a full-dimensional structure until it becomes necessary. This means that if you specify a 2D structure where all regions span the entire simulation domain in the `y`-direction, Sentaurus Process will create a 1D structure.

When a 2D or 3D mask is used in an `etch`, a `deposit`, or a `photo` command, Sentaurus Process automatically extrudes the structure and the mesh into the appropriate dimension and copies the data. This delay of creating a full-dimensional structure can be switched off in the `init` command using the option `!DelayFullD`. To increase the dimension manually, use the `grid` command. If a 2D structure is required, that is, both the `line x` and `line y` commands but no `line z` commands have been specified, `grid 2D` or `grid FullD` will cause a 2D structure to be created.

Similarly, if `line x`, `line y`, and `line z` commands have been specified, `grid 2D` can be used to extrude a 1D structure to two dimensions, and a 1D or 2D structure is extruded to three dimensions using `grid 3D` or `grid FullD`. This functionality also can be used to increase the dimension of structures loaded from files. After the structure has been loaded, `line` commands can be issued and the dimension of the structure will increase automatically when necessary or manually using the `grid` command.

Sentaurus Process does not provide a facility to reduce the dimension of a simulation.

When structures are saved to TDR files (other than TDR restart files), the current maximum dimension as specified with `line` commands is used by default in the file. The dimension of the simulation itself is not affected. To save files in the current dimension, the `!FullD` parameter of the `struct` command can be used (see [Saving Structures on page 44](#)). TDR restart files are always saved in the dimension currently used in the simulation.

---

## Interpolating Field Data From an External Structure File Using the `load` Command

The `load` command can be used to interpolate data from a TDR file onto the current structure (see [load on page 1059](#)). For 1D structures, 1D TDR files are allowed. For 3D structures, 3D TDR files are allowed. However, for 2D structures, either a 2D TDR file or a 3D TDR file is allowed.

When loading a 3D file to a 2D structure, the data on the 2D overlap cross-section, between the 3D structure and the 2D structure, is interpolated to the current 2D mesh. The 2D structure is assumed to be located at  $z=0$ .

## 2: Working With the Simulator

### Saving Structures

Several options can handle the new and old datasets. For example, the `merge` option loads only datasets that do not currently exist in the structure, the `sum` option adds new datasets and sums the matching datasets, the `replace` option adds new datasets and replaces existing datasets with new datasets of the same name, and the `rename` option adds new datasets and renames them by adding the suffix `_load`. These actions also can be applied individually to selected datasets using the `species` and `actions` arguments.

For example, the following command sums `Arsenic_Implant` and the existing `Arsenic_Implant` (if available), and replaces the existing `Damage_Implant` data field by the one in the TDR file:

```
load tdr= in species= {Arsenic_Implant Damage_Implant} actions= {sum replace}
```

The external structure also can be translated or rotated before interpolation with the `transform` argument. This is especially useful when loading 3D data to a 2D structure since the cross section must be at  $z=0$  (the 2D structure is assumed to be allocated at  $z=0$ ). For example, the following command loads the 3D data at  $z=0.5$  instead of  $z=0$ :

```
load tdr= source3d transform= { 1 0 0 0 1 0 0 0 1 0. 0. -0.5 }
```

While the following command loads the 3D data at  $y=0$  since the 3D structure was rotated, and the y-axis and the z-axis were exchanged:

```
load tdr= source3d transform= { 1 0 0 0 0 1 0 1 0 0. 0. 0. }
```

To ensure the transformation is performed correctly, you may save a TDR file for the transformed structure with the `save.transform` argument.

---

## Loading 1D Profiles: The `profile` Command

The `profile` command can load a 1D profile into 1D, 2D, or 3D structures (see [profile on page 1137](#)). The file to be read must contain one x-coordinate data pair per line. Both linear and logarithmic interpolation are available. For example, profiles are loaded using:

```
profile infile= file.dat name= Boron
```

In this case, Sentaurus Process reads the `file.dat` file and sets the `Boron` field accordingly.

---

## Saving Structures

Sentaurus Process uses the TDR file format for saving the structure geometry with and without the bulk mesh and data, and with contacts. TDR files contain simply connected regions to

operate smoothly with other Synopsys TCAD tools. One important option available for saving files is to omit saving gas regions because this may cause problems for other tools.

The TDR format allows you to save and load geometry and data information along with `pdb` parameters (see [File Types on page 14](#)).

TDR files can be used to split a simulation, and to restart and continue the simulation as if no file save or file load was performed. Besides the simulation grid and data, additional information is stored to facilitate such a restart.

**NOTE** It is recommended to set the simulation coordinate system using the `math coord.ucs` command, which specifies the use of the unified coordinate system (UCS). When using the UCS, the visualization coordinates are identical to the simulation coordinates.

To select the fields stored in TDR files, use the `SetTDRList` command. Each field name in the `SetTDRList` command is added to the list of fields, which are usually saved (if the field is present in the structure). This command also takes as arguments the macro parameters `Dopants` and `Solutions`, and their negative counterparts `!Solutions` and `!Dopants`. `Solutions` refers to variables of partial differential equations (PDEs). The solution variables must be stored in a TDR file if that file is to be used to continue a simulation. The parameter `Dopants` refers to the total and active dopant concentration fields. By default, TDR files are saved with both `Solutions` and `Dopants` names in `SetTDRList`. However, this requires many fields to be stored in the TDR files and, sometimes, it is more convenient to have fewer fields.

To do this, set `!Solutions` in `SetTDRList`, which deselects all fields. Then, specify the field names to be stored in the TDR file (see [SetAtomistic on page 1175](#) for saving kinetic Monte Carlo fields).

---

## Saving a Structure for Restarting Simulations

When saving files using the TDR format, the current state of the parameter database is, by default, saved in the file. The parameter database contains all of the information necessary to restart a simulation including:

- Model settings
- Parameter settings
- Geometric tolerance settings
- Refinement boxes from the `refinebox` command
- Temperature ramps from the `temp_ramp` command
- Gas flow specifications from the `gas_flow` command

## 2: Working With the Simulator

### Saving Structures

- Line specifications from the `line` command
- Region specifications from the `region` command
- Reaction specifications from the `reaction` command
- Specifications for `point`, `polygon`, `polyhedron`
- Doping specifications with the `doping` command
- User materials created with the `mater` command
- Contact definitions created with the `contact` command
- Mask definitions created with the `mask` command
- Solution commands can be optionally stored using the `store` parameter of the `solution` command
- Term commands can be optionally stored using the `store` parameter of the `term` command
- Global Tcl variables can be stored with `fset`
- Tcl procedures can be stored using `fproc`

By default, when loading a TDR file, the changes in the parameter database are read in from the TDR file and are applied. For information about the TDR format, refer to the *Sentaurus™ Data Explorer User Guide*.

When saving a TDR file, the simulation coordinate system used is also included in the file and is used by Sentaurus Visual when opening the file.

The visualization coordinate system is the same as the simulation coordinate system. To change the coordinate system, use the `math` command. For the UCS, use:

```
math coord.ucs
```

**NOTE** It is recommended to always use the `math coord.ucs` command.

---

## Saving a Structure for Device Simulation

In general, the main steps to saving a structure appropriate for device simulation are:

1. Define contacts.
2. Remesh the structure with appropriate refinement for device simulation.
3. Save the structure with contacts and with Delaunay weights.

Contacts are defined using the `contact` command. To define contacts, you can either:

- Use a *box* where the contact is created at the intersection of a material interface and a box.
- Use a *region* contact in which a region is specified by giving a point inside the region; then all boundaries of this region become a contact.

The contact is given a name and, if the command is executed multiple times with the same contact and the `add` parameter, the contact will include all parts specified. There are also options for creating a contact on the outer boundaries and so on (see [contact on page 916](#)).

Remeshing the structure is needed to create a mesh that is better suited to device simulation. Typically, this means discarding process-based refinements, creating a very fine mesh under the channel, and refining on the p-n junction. A typical sequence of steps is:

- Clear the process mesh:

```
refinebox clear
line clear
```

- Reset default settings for adaptive meshing:

```
pdbSet Grid AdaptiveField Refine.Abs.Error 1.e37
pdbSet Grid AdaptiveField Refine.Rel.Error 1e10
pdbSet Grid AdaptiveField Refine.Target 100.0
```

- Set high-quality Delaunay meshes:

```
pdbSet Grid SnMesh DelaunayType boxmethod
```

- Set mesh spacing near interfaces:

```
pdbSet Grid SnMesh min.normal.size <n>
pdbSet Grid SnMesh normal.growth.ratio.2d <n>
pdbSet Grid SnMesh normal.growth.ratio.3d <n>
```

- Set which interfaces will have interface refinement:

```
refinebox interface.materials= {Silicon}
```

- Specify adaptive refinement:

```
pdbSet Grid Adaptive 1
```

- Specify lines if necessary:

```
line y loc= $Ymin+0.001
line z loc= $Zmin+0.001
```

- Specify refinement boxes, for example:

```
refinebox min= <list> max= <list> xrefine= <list> yrefine= <list>
zrefine= <list> ;# gate refinement

refinebox refine.fields= NetActive max.asinhdiff= {NetActive= 1.0} \
refine.min.edge= <list> Silicon ;# adaptive refinement on NetActive
```

## 2: Working With the Simulator

### Saving Structures

- If you use the IC WorkBench Edit/View Plus–TCAD Sentaurus interface, it may be helpful to consider using the `mask` argument of the `refinebox` command (see [Chapter 13 on page 835](#) and [refinebox on page 1151](#)).

To save the structure for device simulation, use the command `struct tdr=<c> !Gas`. This command causes a remesh if necessary, stores any contacts that have been defined previously, and includes fields required for device simulation.

Delaunay weights can be saved in the structure intended for device simulation by setting these parameters before generating the mesh:

```
pdbSet Grid SnMesh StoreDelaunayWeight 1  
pdbSet Grid Contacts.In.Brep 1
```

The first parameter `StoreDelaunayWeight` creates the field variable Delaunay–Voronoi weight (`DelVorWeight`) that is used in the weighted box method in Sentaurus Device. The second parameter `Contacts.In.Brep` switches on a feature that creates contacts in the boundary representation (brep) and prevents changes to the mesh that can locally invalidate the Delaunay weight.

---

## Converting Silicon Material to SiGe Material

You can save germanium-doped Silicon material as `SiliconGermanium` material when either:

- The `Skip.Parameter.Interpolation` parameter is switched on and the maximum germanium concentration exceeds `SiliconGermanium.ConversionConc`.

The mole-fraction field, `xMoleFraction`, is generated by the definition of the `BinaryCompounds` parameter when saving a structure. The following commands are set by default:

```
pdbSet Silicon SiliconGermanium.ConversionConc 5E19  
pdbSet Silicon BinaryCompounds {{SiliconGermanium GeTotal "GeTotal/5E22"}}
```

- The `Skip.Parameter.Interpolation` parameter is switched off and the maximum germanium concentration exceeds `TDR.Min.Conv.Conc`, which is set to the same value as `Min.Conv.Conc` by default (see [Defining Alloy Materials on page 28](#)).

**NOTE** Do not set `TDR.Min.Conv.Conc` to a value greater than `Min.Conv.Conc` because TDR still saves the `xMoleFraction` field, which can be generated during the diffusion step.

---

## Saving Doping Information in SiC and GaN for Device Simulations

Basic process simulation capabilities such as etching, deposition, and implantation with Monte Carlo are available for multicomponent materials, for example, silicon carbide (SiC) and gallium nitride (GaN). However, there are no activation models for some of the dopants in these materials, while the activation of some dopants (for example, boron) in SiC is determined by solid solubility. To create proper active doping concentration fields, when saving a file for transfer to device simulation, use the `diffuse` command with zero time and proper diffusion temperature, for example:

```
diffuse time= 0 temperature= 2100
struct tdr= filename
```

---

## Saving 1D Profiles for Inspect

To store .plx files, use the `WritePlx` command. The command `SetPlxList` selects the fields to be stored in the .plx file. The `SetPlxList` command is similar to the `SetTDRList` command, except that no fields are selected by default. Only the field names specified in `SetPlxList` are stored in the .plx file (see [SetPlxList on page 1186](#) and [WritePlx on page 1256](#)).

---

## Saving 1D TDR Files From 2D and 3D Simulations, and 2D TDR Files From 3D Simulations

The command `struct` also saves a 1D TDR file if the proper cutting coordinates are specified (see [struct on page 1217](#)). In two dimensions, only one cutting coordinate is needed (either x or y; the z-coordinate makes no sense here). In three dimensions, the command saves the intersection of the planes specified by two cutting coordinates (for example, specifying x and z will save the y line containing those x- and z-coordinates). In addition to storing the mesh and data, these files save any contacts that apply at the cut point, so that the file can be loaded into Sentaurus Device for electrical analysis. This file can be visualized with Sentaurus Visual.

For 3D simulations, the `struct` command also saves 2D TDR files when one cutting coordinate is specified.

For example, in a 2D simulation, the following command picks up all the x-coordinates with  $y=0.5$  and saves them in a 1D TDR file:

```
struct tdr= filename y= 0.5
```

## 2: Working With the Simulator

### Saving Structures

In addition, in a 3D simulation, the following command saves the y-coordinates with  $x=0.2$  and  $z=0.1$  as a 1D TDR file:

```
struct tdr= filename x= 0.2 z= 0.1
```

The following command saves a 2D cross section of the 3D structure to a 2D TDR file at  $x=0.2$ :

```
struct tdr= filename x= 0.2
```

---

## The select Command (More 1D Saving Options)

The `select` command is a versatile command for many operations such as viewing results, postprocessing, and initializing or changing datasets. The basic command is:

```
select z=<c>
```

where `<c>` is an Alagator expression (see [Chapter 7 on page 603](#)). A simple example of an expression is the name of a data field such as `Potential` and `vTotal`. The value of the expression is stored in the selected field.

This selected field can be viewed with `print.data` or `print.1d`, for example, or the integrated values can be obtained using the `layers` command. The `select` command can also be used to set an existing data field or create a new data field, for example:

```
select z= 1.0 name= MyDataField ;# create a new data field named MyDataField  
;# and set it to 1.0 (everywhere)  
select z= 0.1*Vacancy name= Void store ;# Set Void equal to 0.1*Vacancy
```

---

## The datexcodes.txt File

The `datexcodes.txt` file is the Synopsys configuration database for materials, doping species, and other quantities that are used in semiconductor process and device simulations. Sentaurus Process uses this file in two ways:

- The "floops" property of each field is read in and is used as a conversion factor between short internal names and proper DATEX names expected by other tools.
- The unit field is read from the `datexcodes.txt` file and is used to convert internal units to those units expected by other tools.

For example, the distributed `datexcodes.txt` file contains the following field definition:

```
VacancyConcentration {  
    label      = "total Vacancy concentration"  
    symbol     = "VTotal"
```

```
unit      = "cm^-3"
factor    = 1.000E+12
precision = 4
interpol  = arsinh
material  = All
alter1    = vacancy
alter2    = 0
property("floops") = "VTotal"
}
```

From this definition, Sentaurus Process reads property("floops") to enable conversion of the internally named field VTotal to VacancyConcentration in the TDR file and to save VacancyConcentration in cm<sup>-3</sup>.

---

## References

- [1] B. B. Welch, *Practical Programming in Tcl & Tk*, Upper Saddle River, New Jersey: Prentice Hall PTR, 3rd ed., 2000.

## **2: Working With the Simulator**

References

*The chapter describes how ion implantation is implemented in Sentaurus Process.*

---

## Overview

Ion implantation is a widely used processing technique to introduce impurity atoms into semiconductor materials. In Sentaurus Process, either analytic functions or the Monte Carlo (MC) method can be used to compute the distribution of implanted ions and the implantation damage.

Analytic implantation models use the simple Gaussian and Pearson functions as well as the advanced dual-Pearson functions. The algorithms for analytic implantation are integrated in Sentaurus Process. The implantation damage with analytic models is calculated according to the Hobler model [1].

The MC method uses a statistical approach to calculate the penetration of implanted ions into the target and the accumulation of crystal damage based on the binary collision approximation (BCA) [2]. The engine for MC implantation is Sentaurus MC [3].

Sentaurus Process handles 1D, 2D, and 3D geometries for both analytic implantation and MC implantation. The algorithms for analytic implantation are an integral part of Sentaurus Process; whereas, MC implantation is performed based on the BCA.

Analytic implantation simulates the spatial distribution of implanted ions based on the selected distribution function, which is described by *moments*. The distribution moments depend on the ionic species, implantation energy, dose, tilt angle, and rotation angle. Sets of moments for a given range of implantation parameters are provided in the form of lookup tables. Sentaurus Process can use different implantation tables in various formats.

Both analytic implantation and MC implantation are performed using the `implant` command (see [implant on page 1001](#)). There are two aspects to using the `implant` command: selecting models and parameters, and then running the simulation.

**NOTE** In most cases, you do not need to select models and parameters. Sentaurus Process makes the selection automatically. You should select models using the `implant` command only if you are an advanced user.

### 3: Ion Implantation

#### Working With Ion Implantation

---

## Working With Ion Implantation

This section presents how to implement an ion implantation.

### Specifying Analytic or Monte Carlo Implantation

Analytic implantation is performed using the `implant` command. At its simplest, you can use:

```
implant <species> energy=<n> dose=<n> tilt=<n> rotation=<n>
```

See [Analytic Implantation on page 62](#).

To switch from analytic implantation to MC implantation using Sentaurus MC, use:

```
implant <species> energy=<n> dose=<n> tilt=<n> rotation=<n> sentaurus.mc
```

If `cascades` is specified in addition to `sentaurus.mc`, the MC implantation is run in full-cascade mode:

```
implant <species> energy=<n> dose=<n> tilt=<n> rotation=<n> sentaurus.mc \
cascades
```

See [Monte Carlo Implantation on page 107](#).

A previously generated MC implantation profile can be loaded using `load.mc`:

```
implant <species> energy=<n> dose=<n> tilt=<n> rotation=<n> load.mc file=<c>
```

A TDR file must be specified using the `file` argument. The `load.mc` option works with files created by Sentaurus MC. See [Loading External Profiles on page 163](#).

### Specifying Implantation Parameters

The implantation energy is given in keV by default.

The implantation dose has two modes:

- The wafer dose (`WaferDose`) refers to the expected dose in the structure after the implantation is finished. This dose is measured in ions per  $\text{cm}^2$ .
- The beam dose (`BeamDose`).

In the wafer dose mode, the final implanted dose does not depend on the wafer orientation with respect to the ion beam. In the beam dose mode, the final implanted dose may change as the

tilt angle and the rotation angle change. All angles are measured in degrees. For more information, see [Coordinate System for Implantation: Tilt and Rotation Angles on page 59](#).

The mode of the implanted dose can be specified with the following switches:

```
pdbSet ImplantData DoseControl {Default WaferDose BeamDose}
```

The default value of `DoseControl` is `Default`, in which case, the mode of the implanted dose is chosen automatically based on the implantation table format. If the currently selected implantation tables are in Taurus™ or TSUPREM-4™ format, the beam dose mode is used automatically. Otherwise, the wafer dose mode is applied. If `DoseControl` is set to `WaferDose`, the wafer dose mode is used for all implantations regardless of table formats, likewise for `BeamDose`.

**NOTE** To obtain consistent results and to prevent an unexpected dose mode, it is strongly recommended to always set `DoseControl` at the start of command files to either `WaferDose` or `BeamDose`.

To override these global settings, use `beam.dose` in the `implant` command:

```
implant <species> dose=<n> beam.dose
```

**NOTE** The main implantation parameters – energy, dose, tilt, and rotation of the `implant` command – must always be specified. Otherwise, default values are chosen that may not reflect the assumed process conditions.

In addition to `energy`, `dose`, `tilt`, and `rotation`, you can specify the implantation temperature and the dose rate. Temperature and dose rate are recognized as parameters by the format moment tables of Taurus Process.

If the structure is completely covered by photoresist, you can omit an implantation step by using the following command:

```
pdbSet ImplantData ResistSkip 1
```

By default, the implantation step is not omitted.

The amount of information displayed and printed to the log file is controlled by the common optional argument `info`, which can be specified in the `implant` command (see [Common Arguments on page 899](#)).

### 3: Ion Implantation

#### Working With Ion Implantation

---

## Selecting Models

The implanted species must be a previously initialized species. To initialize an implantation species, use:

```
implant species=<c> <material> [imp.table=<c>] [damage]
[dualpearson | gaussian | pearson | pearson.s | point.response]
```

where `species` can be any name, and `<material>` must be an initialized material (see [Specifying Materials on page 18](#)).

**NOTE** This `implant` command does not perform an implantation. It is distinguished by the argument `species` (or `tables`).

At the beginning of a Sentaurus Process run, all species are initialized automatically using `species=<c>`.

To select an implantation table containing moments for the primary and lateral distributions, use `imp.table`.

As previously mentioned, it is not necessary to select the implantation model since this is performed automatically. If required, you can specify explicitly one of the available implantation models (see [Primary Distribution Functions on page 63](#)).

To switch on damage calculation based on the Hobler model, use the `damage` option.

For example, the following command changes the default implantation table for boron in silicon to `my_table.tab`, changes the implantation model to single Pearson, and switches off the damage calculation for boron in silicon:

```
implant species= Boron Silicon imp.table= my_table.tab pearson !damage
```

[Table 5 on page 57](#) lists the species that are initialized and supported in a Sentaurus Process run. If you want to implant an unknown species, you can define a new species by first setting its atomic number and atomic mass using PDB commands:

```
pdbSetDouble ImplantData <species> AtomicNumber <n>
pdbSetDouble ImplantData <species> AtomicMass <n>
```

Then, initialize the new species using the `implant` command:

```
implant species=<c> Silicon
```

Now you can perform a MC implantation for this newly defined species like any other built-in species. For analytic implantation, you also need to select the implantation model and to set the implantation table for the new species.

Table 5 Species initialized and supported by Sentaurus Process

Atomic species	Molecular species	Description
Aluminum, Antimony, Arsenic, Boron, Carbon, Fluorine, Gallium, Germanium, Indium, Nitrogen, Phosphorus, Silicon	AsH <sub>2</sub> , BF <sub>2</sub> , B <sub>10</sub> H <sub>14</sub> , B <sub>18</sub> H <sub>22</sub> , BC <sub>12</sub> , C <sub>2</sub> B <sub>10</sub> H <sub>12</sub> , C <sub>2</sub> B <sub>10</sub> H <sub>14</sub> , PH <sub>2</sub>	Used in analytic and MC implantations. Implantation tables are available for atomic species and molecular BF <sub>2</sub> . For other molecular species, implantation is performed based on the tables for the primary dopant species (As, B, or P).
Argon, Beryllium, Bromine, Cadmium, Chlorine, Helium, Hydrogen, Iodine, Iron, Krypton, Lead, Magnesium, Neon, Oxygen, Selenium, Sulfur, Tellurium, Tin, Titanium, Xenon, Zinc		No implantation tables are available. Analytic implantation will terminate. Recommended for MC implantations only.

You can overwrite or extend these settings at any time during a Sentaurus Process run. There are three principal ways to change the initial settings.

With the previously described command, you can change the settings for *one* pair of dopant species and material.

To overwrite the settings for *one* particular dopant species in *all* materials, use:

```
implant [species=<c>] tables= Default | Dios | Tasch | Taurus | TSuprem4
```

Internally, Sentaurus Process executes a set of `implant species=<c> <material>` commands, which set the implantation parameters for one pair of dopant species and material, respectively.

**NOTE** The `tables` argument does not refer to a particular table or table name. It sets all tables and model switches for the species in all materials using a Tcl procedure.

The available options for `tables` are discussed in [Implantation Tables on page 74](#).

## Simulating Multirotation Implantations

To simulate multirotation implantations for both the analytic functions and the MC method, use `mult.rot=<i>`. If `mult.rot` is set to an integer greater than 1, an implantation with a revolving ion beam is simulated. Starting with the user-defined rotation angle, Sentaurus Process performs multirotation implantations with the same energy and tilt in one `implant` command.

### 3: Ion Implantation

#### Working With Ion Implantation

The rotation angle is incremented by  $360^\circ / \text{mult.rot}$  and, for each implantation step, the dose is the  $1/\text{mult.rot}$ -th part of the user-specified dose.

---

## Simulating Energy Contamination Implantations

Sentaurus Process can perform implantations with energy contamination, in which a fraction of the nominal dose has a different energy from the specified energy.

To perform an energy contamination implantation, you must specify `contamination` in the `implant` command. The syntax is:

```
implant dose=<n> energy=<n> contamination= {energy=<n1> dose.fraction=<n2>}
```

Sentaurus Process treats the implantation as two separate implantations in the following order:

```
implant dose=<n*n2> energy=<n1> ...
implant dose=<n*(1-n2)> energy=<n> ...
```

---

## Specifying Adaptive Meshing During Implantation

Adaptive meshing during implantation is active whenever adaptive meshing is switched on, that is, `pdbGet Grid Adaptive` returns a 1.

It also can be switched on by specifying `Adaptive` in the `implant` command (see [Adaptive Meshing During Implantation on page 738](#)).

In addition, the `mult.rot.adaptive` argument of the `implant` command allows you to switch on or off adaptive remeshing in certain rotations in multirotation implantations. The `mult.rot.adaptive` argument takes a list of Boolean switches (0 or 1). The number of Booleans in this list must be the same as `mult.rot=<i>`. If the number of Booleans specified is less than `<i>`, the remaining Booleans are assumed to be the same as the main adaptive switch. That is, if adaptive remeshing (`Adaptive` in the `implant` command or the PDB parameter `Grid Adaptive`) is true, the unspecified switches in the `mult.rot.adaptive` list are also true. On the other hand, if adaptive remeshing is false, the unspecified switches in the `mult.rot.adaptive` list are also false.

In general, since analytic implantation and MC implantation produce similar results, MC implantation can use this similarity for adaptive meshing.

When adaptive meshing is active, MC implantation first calls analytic implantation for mesh refinement. At the end of the analytic implantation, the concentration generated by the analytic implantation is discarded, while the new mesh is used for MC implantation.

If the analytic implantation fails for whatever reason (for example, there are no implantation tables for certain materials), Sentaurus Process issues a warning, and the MC implantation proceeds with the original mesh.

---

## Coordinate System for Implantation: Tilt and Rotation Angles

Regardless of whether a simulation is 1D, 2D, or 3D, the direction of the ion beam is defined relative to the wafer coordinate system (see [Figure 5 on page 37](#)) by the values of the `tilt` and `rotation` arguments of the `implant` command. [Figure 8](#) shows the tilt and rotation angles in the wafer coordinate system.

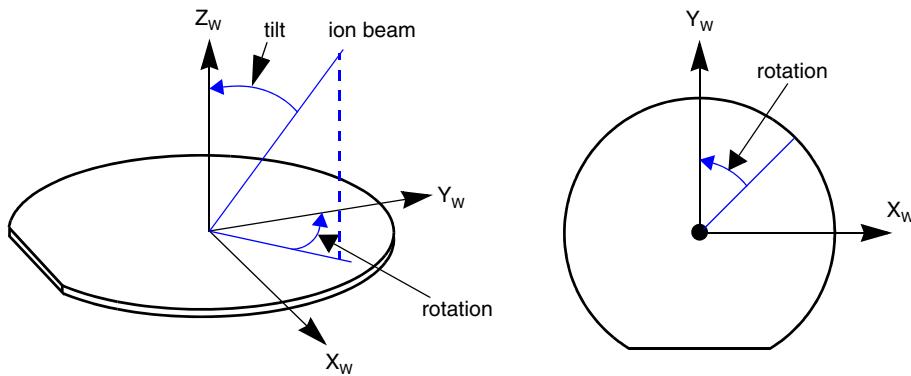


Figure 8 Tilt and rotation angles for implantation; beam angle shown corresponds to  
tilt= 20 and rotation= 45

The tilt and rotation angles are measured from the ion beam to the wafer z-axis and the wafer y-axis, respectively. In this definition, the tilt angle is always positive, and between 0° (inclusive) and 90°. However, for convenience, a negative tilt angle is allowed, and it is converted automatically to a positive tilt by adding 180° to the specified rotation angle. The rotation angle is positive when the beam is rotated in a clockwise direction about the wafer z-axis, and it is negative when the beam is rotated counterclockwise.

Since the tilt and rotation angles are measured with respect to the wafer axes, the direction of the beam in the simulation coordinate system depends on the slice angle.

### 3: Ion Implantation

#### Coordinate System for Implantation: Tilt and Rotation Angles

Figure 9 shows the relationship between wafer coordinates, simulation coordinates, and the beam direction.

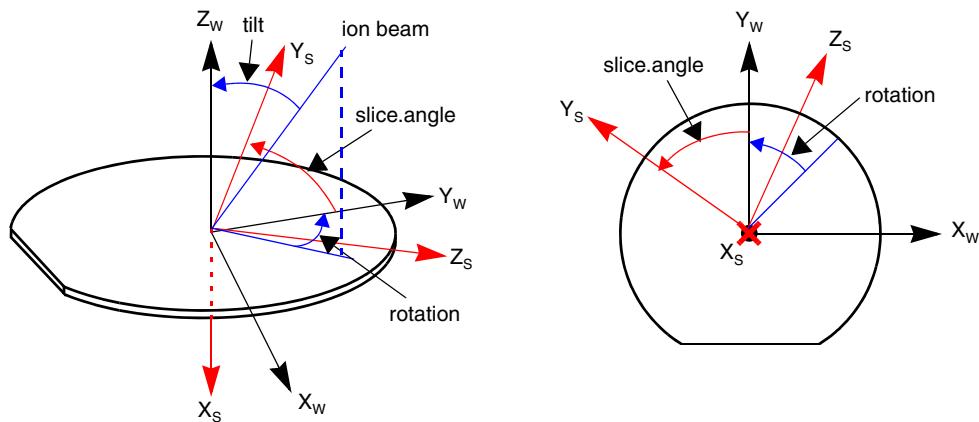


Figure 9 Tilt and rotation angles for implantation; angles shown correspond to tilt= 20, rotation= 45, and slice.angle= 60

The default values of `tilt` and `rotation` are  $7^\circ$  and  $-90^\circ$ , respectively; in other words, by default the incident ion beam is directed parallel to the wafer flat tilted away from the wafer x-axis. For the default slice angle of  $-90^\circ$  (specified in the `init` command), this corresponds to an ion beam in the simulator xy plane, tilted away from the simulator y-axis. In a 2D simulation, the default ion beam comes from the left side.

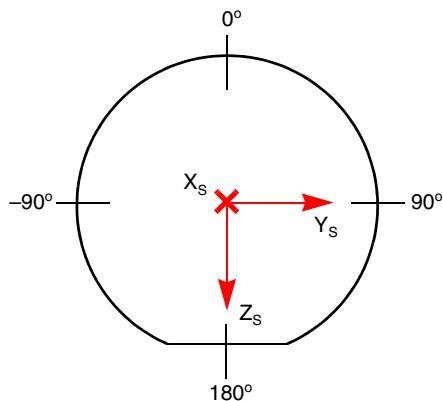


Figure 10 Implantation rotation directions for positive tilt

Figure 10 shows the projection into the wafer plane of the direction from which the beam strikes the wafer for `tilt` > 0 and various rotation angles. The default simulation coordinate system (`slice.angle=-90`) is also shown.

[Figure 11](#) shows clearly that the orientations shown in [Figure 10 on page 60](#) are consistent with the conventions defined in [Figure 8 on page 59](#). A rotation of  $90^\circ$  corresponds to rotating the wafer a quarter turn counterclockwise.

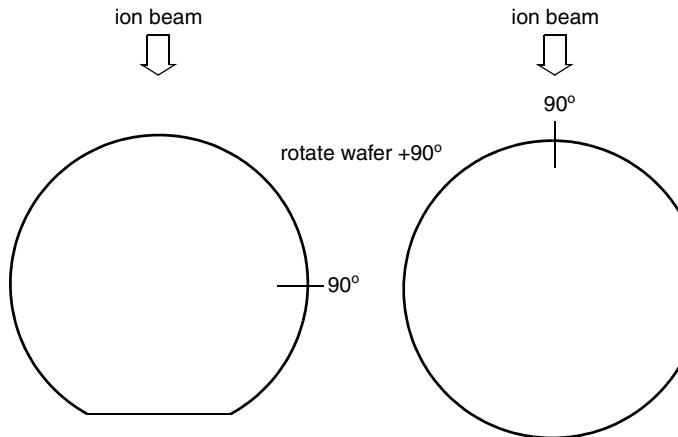


Figure 11 Rotating wafer and fixed beam direction

## 2D Coordinate System

In a 2D simulation, the orientation of the 2D simulation plane with respect to the wafer coordinate system must be defined. The angle between the 2D simulation plane and the y-axis is set by `slice.angle` in the `init` command (see [init on page 1020](#)). Its default value of  $-90^\circ$  orients the 2D simulation plane parallel to the wafer flat. The transformed y-axis ( $y_s$ ) is the y-axis in the 2D simulation plane.

To set `slice.angle`, you can either:

- Set it directly:

```
init slice.angle=<n>
```

- Set it by specifying a 2D cutline (see [CutLine2D on page 924](#)):

```
init slice.angle= [CutLine2D <x1> <y1> <x2> <y2>]
```

where `<x1>` and `<y1>` define the start point, and `<x2>` and `<y2>` define the end point in the wafer plane. The two points are in the wafer coordinate system (see [Wafer Coordinate System on page 37](#)).

**NOTE** To make a TCAD layout compatible with the `slice.angle`, use the following commands:

```
set SliceAngle -90
set SliceOffset [icwb slice.angle.offset]
init slice.angle= [expr $SliceAngle+$SliceOffset]
```

### 3: Ion Implantation

#### Analytic Implantation

In general, the tilt projected into the 2D simulation plane is different from the `tilt` value. It is given by the geometric relation:

$$\cos(\text{tilt}2\text{D}) = \frac{\cos(\text{tilt})}{\sqrt{\cos^2(\text{tilt}) + \sin^2(\text{tilt}) \cdot \cos^2(\text{rotation} + \text{slice.angle})}} \quad (7)$$

The angle `tilt2D` can be found in the output of Sentaurus Process and can be negative depending on the rotation angle and slice angle.

The `tilt` value defines the relation between the wafer dose (`dose`), given on the command line by default, and the dose, which must be specified in the beam dose mode to obtain the same final implanted dose, that is:

$$\text{BeamDose} = \frac{\text{dose}}{\cos(\text{tilt})} \quad (8)$$

`BeamDose2D` as it appears in the Sentaurus Process output is defined using `tilt2D`, that is:

$$\text{BeamDose2D} = \frac{\text{dose}}{\cos(\text{tilt}2\text{D})} \quad (9)$$

---

## Analytic Implantation

Analytic implantation is performed using empirical point-response distributions, which are generated using moments. The moments representing the primary and lateral point-response functions are taken from implantation tables.

For 2D simulations based on analytic functions, an ion beam incident at the point  $(\xi, \eta)$  is assumed to generate a distribution function  $F(x, y, \xi, \eta)$ .

To calculate the concentration of the implanted species at a point  $(x, y)$  of the simulation domain, the superposition of all distribution functions of all possible points of incidence  $(\xi(s), \eta(s)) \in \Gamma_{\text{gas}}$  must be computed:

$$C(x, y) = N_d \int_{\Gamma_{\text{gas}}} F(x, y, \xi(s), \eta(s)) ds \quad (10)$$

where  $N_d$  is the total dose per exposed area, and  $C(x, y)$  is the doping profile.

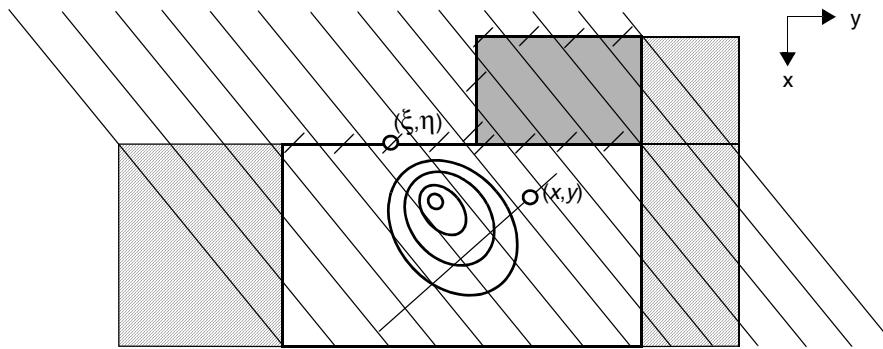


Figure 12 Point-response distribution for a particle incident at the point  $(\xi, \eta)$  at the surface; intervals are used for lateral integration at the point  $(x, y)$ ; shaded regions to left and right mark the lateral extension elements

The 2D distribution functions are always assumed to be given as a product of two 1D distribution functions orthogonal to each other: a primary distribution function  $f_p(x)$  and a lateral distribution function  $f_l(y)$ :

$$F(x, y, \xi, \eta) = f_p(x - \xi(s)) \cdot f_l(y - \eta(s)) \quad (11)$$

To compute the convolution integral in two dimensions, Sentaurus Process uses a set of lateral intervals perpendicular to the projected ion beam. A local 1D layer structure is computed in each interval. The spacing and the width of these intervals depend on the complexity of the exposed gas surface.

In three dimensions, Sentaurus Process uses a slightly different algorithm. The point-response function is a 3D function. The lateral function  $f_l(z)$  also is used in the third direction, assuming an axially symmetric point-response function:

$$F(x, y, z, \xi, \eta, \Theta) = f_p(x - \xi(s)) \cdot f_l(y - \eta(s)) \cdot f_l(z - \Theta(s)) \quad (12)$$

The lateral integration is performed in the plane perpendicular to the ion beam. For each point in the lateral integration plane, again, a local 1D layer structure is computed.

## Primary Distribution Functions

Primary distribution functions can be set for a species–material combination using:

```
implant species=<c> <material>
[dualpearson | gaussian | pearson | pearson.s | point.response]
```

The previous model selection is used if no model selection is made.

### 3: Ion Implantation

#### Analytic Implantation

The primary distribution is used to represent the point-response function in one dimension, or the vertical point-response in two dimensions and three dimensions. Point-response functions are characterized by moments.

The first moment, the projected range  $R_p$ , is defined as:

$$R_p = \int_{-\infty}^{\infty} x \cdot f(x) \cdot dx \quad (13)$$

The higher moments  $m_i$  are defined as:

$$m_i = \int_{-\infty}^{\infty} (x - R_p)^i \cdot f(x) \cdot dx \quad (14)$$

The standard deviation  $\sigma$ , the skewness  $\gamma$ , and the kurtosis  $\beta$  are defined as:

$$\begin{aligned} \sigma &= \sqrt{m_2} \\ \gamma &= \frac{m_3}{\sigma^3} \\ \beta &= \frac{m_4}{\sigma^4} \end{aligned} \quad (15)$$

## Dual-Pearson Distribution: dualpearson

The most advanced primary distributions are available with the dual-Pearson function [4]. The dual-Pearson model includes a superposition of two Pearson functions:

$$f_p(x) = \text{ratio} \cdot f_{\text{head}}(x) + (1 - \text{ratio}) \cdot f_{\text{tail}}(x) \quad (16)$$

The head and tail functions are two independent Pearson functions. The head function accounts for the profile of ions that do not channel (nonchanneling or amorphous part). The tail function accounts for the channeled ions that form the characteristic tail in the implantation profile.

A dual-Pearson function is characterized by nine parameters: the two sets of four Pearson parameters and the ratio between the amorphous and channeling doses. These parameters are usually taken from moment table files.

You can set the individual moments directly on the command line, for example:

```
implant species=<c> <material> [rp=<n>] [stdev=<n>] [gamma=<n>]
[beta=<n>] [rp2=<n>] [stdev2=<n>] [gamma2=<n>] [beta2=<n>] [ratio=<n>]
[lat.stdev=<n>] [lat.stdev2=<n>]
```

This overwrites the parameters found in the specified implantation table. It is also possible to force the Pearson distributions in the dual-Pearson and Pearson models to behave like a Gaussian distribution, for example:

```
implant species= Boron Silicon pearson gamma= 0 beta= 3
```

The first statement sets the implantation model to a Pearson distribution. The parameters are read from the default table. The skewness and the kurtosis are set according to [Eq. 18](#), overwriting the values found in the table. This results in a Gaussian distribution for the function characterizing the amorphous part of the profile.

You can enable or disable individual moments using `<moment>.isset` switches, where `<moment>` is the name of the moments such as `rp`, `stdev`, `rp2`, and `stdev2`. For example, to disable a user set value for `rp`, use:

```
pdbSetBoolean Silicon Boron rp.isset 0
```

**NOTE** All moments set on the command line are ignored after a new implantation table is selected, or an implantation table has been specified again using the `implant species=<c> <material> imp.file=<c>` command. In this case, the moments from this new implantation table will be used, regardless of which moments have been set previously on the command line.

## Gaussian Distribution: gaussian

$$f_p(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-R_p)^2}{2\sigma^2}\right) \quad (17)$$

$$\begin{aligned} \gamma &= 0 \\ \beta &= 3 \end{aligned} \quad (18)$$

### 3: Ion Implantation

#### Analytic Implantation

## Pearson Distribution: pearson

The Pearson distributions are the solution to the following differential equations:

$$\begin{aligned}
 \frac{d}{dy} f(y) &= \frac{y - a}{b_0 + b_1 \cdot y + b_2 \cdot y^2} \cdot f(y), \quad y = x - R_p \\
 a = b_1 &= -\frac{\gamma \cdot \sigma \cdot (\beta + 3)}{A} \\
 b_0 &= -\frac{\sigma^2 \cdot (4\beta - 3\gamma^2)}{A} \\
 b_2 &= -\frac{2\beta - 3\gamma^2 - 6}{A} \\
 A &= 10\beta - 12\gamma^2 - 18
 \end{aligned} \tag{19}$$

Different types of Pearson distribution are distinguished by different values of  $\gamma$  and  $\beta$ :

$$\begin{aligned}
 0 < \gamma < 32 \\
 \beta > \frac{48 + 39\gamma^2 + 6(\gamma^2 + 4)^{3/2}}{32 - \gamma^2} \quad \text{Type IV}
 \end{aligned} \tag{20}$$

$$\begin{aligned}
 0 < \gamma < 32 \\
 \beta = \frac{48 + 39\gamma^2 + 6(\gamma^2 + 4)^{3/2}}{32 - \gamma^2} \quad \text{Type V}
 \end{aligned} \tag{21}$$

$$\begin{aligned}
 0 < \gamma < 32 \\
 3 + 1.5 \cdot \gamma < \beta < \frac{48 + 39\gamma^2 + 6(\gamma^2 + 4)^{3/2}}{32 - \gamma^2} \quad \text{Type VI}
 \end{aligned} \tag{22}$$

The Pearson–IV distribution is given by:

$$f_p(y) = K |b_2 y^2 + b_1 y + b_0|^{-\frac{1}{2b_2}} \cdot \exp\left(-\frac{\frac{b_1}{b_2} + 2a}{\sqrt{4b_2 b_0 - b_1^2}} \operatorname{atan}\left(\frac{2b_2 y + b_1}{\sqrt{4b_2 b_0 - b_1^2}}\right)\right) \tag{23}$$

Sentaurus Process automatically switches between the Pearson–IV, Pearson–V, and Pearson–VI distribution functions depending on the conditions for  $\gamma$  and  $\beta$  given in Eq. 20 to Eq. 22. The factor  $K$  is chosen to fulfill the normalization condition:

$$\int_{-\infty}^{\infty} f_p(x) dx = 1 \tag{24}$$

## Pearson Distribution With Linear Exponential Tail: pearson.s

A linear exponential tail is added to the Pearson distribution. This is performed in an attempt to describe more accurately the profile tails for some implantations, that is:

$$f_p(x) = \begin{cases} P_p(x), & 0 \leq x < x_{\max} \\ P_v(x), & x_{\max} < x \leq x_a \\ P_l(x), & x_a \leq x < \infty \end{cases} \quad (25)$$

where  $P_p$  is the Pearson distribution,  $P_v$  is a transition function, and  $P_l$  is the exponential tail.

The decay length of the exponential tail is give by the parameter  $l_{\exp}$ :

$$\begin{aligned} x_{\max}: P_{\max} &:= P_p(x_{\max}) = \max P_p(x) \\ x_a \geq x_{\max}: P_a &:= P_p(x_a) = \frac{1}{2} P_p(x_{\max}) \\ P_v(x) &= P_p(x_{\max}) \cdot \exp(A_1(x - x_{\max})^2 + B(x - x_{\max})^3) \\ P_l(x) &= P_p(x) + \frac{x - x_{\max}}{l_{\exp}} \cdot P_p(x_{\max}) \cdot \exp\left(-\frac{x - x_{\max}}{l_{\exp}}\right) \end{aligned} \quad (26)$$

The constants  $A_1$  and  $B$  are computed from the continuity conditions:

$$P_l(x_a) = P_v(x_a) \quad (27)$$

and:

$$\begin{aligned} \frac{d}{dx} P_l(x) \Big|_{x_a} &= \frac{d}{dx} P_v(x) \Big|_{x_a} =: P'_a \\ A_1 &= \frac{3 \ln \frac{P_a}{P_{\max}}}{(x_a - x_{\max})^2} - \frac{P'_a}{P_a(x_a - x_{\max})} \\ B &= \frac{-2 \ln \frac{P_a}{P_{\max}}}{(x_a - x_{\max})^3} + \frac{P'_a}{P_a(x_a - x_{\max})^2} \end{aligned} \quad (28)$$

**NOTE** Exponential tail distributions are available with the Dios tables. However, care is required when using the exponential tail for implantation with large tilt angles. The  $l_{\exp}$ -fit in these tables was performed for a standard  $7^\circ$  tilt in amorphous materials and does not apply to large tilt angles or strong channeling conditions.

### 3: Ion Implantation

#### Analytic Implantation

## Point-Response Distribution: point.response

See [Point-Response Interface on page 89](#).

---

## Screening (Cap) Layer-Dependent Moments

Cap layer-dependent implantation tables are used to describe correctly the screening of the ion beam in the structure. The implantation moments in a particular region generally depend on the combined thickness of all layers above this region. The moments are parameterized with respect to the effective thickness  $t_i^{\text{cap}}$ , which is defined as:

$$t_i^{\text{cap}} = \sum_j^{j < i} t_j f_j^{\text{eff}} \quad (29)$$

that is, as the sum over the thicknesses of all layers above the current layer multiplied by the corresponding efficiency factors  $f_j^{\text{eff}}$ . These factors can be set for a particular material and a species using:

```
implant species= Boron Oxide eff.caplayer.thick= 1.0
```

The default value is 1 for all materials other than silicon, where it is set to zero. Therefore, silicon layers are effectively not included in the total effective cap layer thickness.

If the implantation table for a specific species–material combination does not contain an explicit cap layer dependency, the effective channeling suppression model is used. This model suppresses the channeling tail by multiplying the channeling part in [Eq. 29](#) by a factor  $r_{\text{suppress}}$  calculated according to:

$$r_{\text{suppress}} = \frac{1}{\frac{1}{2} \cdot \frac{C(R_p, \text{head})}{C(R_p, \text{head}) + C(R_p, \text{tail})} + \left( \frac{\text{MinRatio}}{\sigma} \right)^{-\text{Exponent}}} \quad (30)$$

where  $C(R_p, \text{head})$  and  $C(R_p, \text{tail})$  are the peak concentrations of the unscaled profile, and  $\sigma$  is defined as:

$$\sigma = \sum_i \frac{t_i}{R_{pi}} \quad (31)$$

using the values of  $R_p$  for the amorphous (head) part of the profile for all layers  $i$  above the present layer. The amorphous part of the profile is multiplied by  $1 - r_{\text{suppress}}$  to conserve the total dose.

MinRatio is the minimum value of the ratio  $\sigma$ . The parameters MinRatio and Exponent can be set in the parameter database, that is:

```
pdbSet <material> <species> MinRatio
pdbSet <material> <species> Exponent
```

The model is applied only for values of  $\sigma$  greater than MinRatio and for an effective cap layer thickness greater than 2.1 nm. The effective channeling suppression model can be switched on using:

```
implant species=<c> <material> eff.channeling.suppress
```

The model remains inactive for explicitly cap layer-dependent implantation tables.

**NOTE** This model is switched off by default and is switched on in the Taurus or TSUPREM-4 mode.

## Lateral Straggle

The lateral straggling of the distribution of implanted ions is specified by defining a lateral distribution function, which is a Gaussian distribution with a lateral standard deviation  $\sigma_l$ :

$$f_l(x, y) = \frac{1}{\sqrt{2\pi}\sigma_l(x)} \exp\left(-\frac{y^2}{2\sigma_l^2(x)}\right) \quad (32)$$

In general, the lateral standard deviation depends on the vertical depth of the profile. The depth dependency can be switched on or off for a particular combination of dopant species and material using depth.dependent:

```
implant species=<c> <material> depth.dependent
```

The lateral standard deviation also can be set in the implant command using lat.stdev:

```
implant species=<c> <material> [lat.stdev=<n>] [lat.stdev2=<n>]
```

where lat.stdev2 sets the lateral standard deviation for the tail function. If either lat.stdev or lat.stdev2 is set, Sentaurus Process switches to depth-independent lateral straggling. All depth.dependent flags are ignored in this case.

An additional scaling factor for both the depth-dependent and depth-independent lateral standard deviation can be used to vary the lateral straggling:

```
implant species=<c> <material> [lat.scale=<n>] [lat.scale2=<n>]
```

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## Depth-Dependent Lateral Straggle: Sentaurus Process Formulation

If a TSUPREM-3-compatible implantation table is used (.s3), the depth-dependent lateral standard deviation is calculated according to:

$$\sigma_l(x) = \text{lstdev} \cdot \exp\left(-\frac{x}{\text{lstdev} \cdot \text{lv}}\right) \quad (33)$$

where `lstdev` and `lv` are parameters taken from the implantation table. There are two independent sets of parameters for the two Pearson functions in the dual-Pearson model. This formulation also is used with the Tasch implantation tables.

## Depth-Dependent Lateral Straggle: Dios Formulation

If a Dios-compatible implantation table is used, the depth-dependent lateral standard deviation is calculated using a vector of five parameters (`p1`, `p2`, `p3`, `p4`, `p5`). The following formula is applied [5]:

$$\sigma_l(x) = \text{stdev} \cdot \max\left(0.01, \frac{\log\left(\exp\left(p1 \cdot \left(\frac{p2 \cdot x}{R_p} + p3\right)\right) + \exp\left(p1 \cdot \left(\frac{p4 \cdot x}{R_p} + p5\right)\right)\right)}{p1}\right) \quad (34)$$

There is only one set of these parameters in each table entry. In the case of the dual-Pearson implantation model (see Eq. 35), the same set of parameters (`p1`, `p2`, `p3`, `p4`, `p5`) together with the standard deviation of the first Pearson function described by `stdev` is applied to both the amorphous and the channeling part of the distribution.

## Depth-Dependent Lateral Straggle: Taurus Formulation

If an implantation table compatible with TSUPREM-4 or Taurus is used, the depth-dependent lateral standard deviation is calculated using two parameters:

$$\sigma_l(x) = \sigma_0 \cdot \left(1 + \Delta\sigma \left(\frac{x}{R_p} - 1\right)\right) \quad (35)$$

The depth-independent standard deviation  $\sigma_0$  and the depth-dependent slope  $\Delta\sigma$  are read from the moment table.

This formulation is compatible with the Dios formulation (see [Depth-Dependent Lateral Straggle: Dios Formulation on page 70](#)) for the following conditions:  $p4 = 0$ ,  $p1 \cdot p5 = -\infty$ . The remaining parameters can be translated as follows:

$$\begin{aligned}\sigma_0 &= \text{stdev} \cdot (p2 + p3) \\ \Delta\sigma &= \frac{p2}{p2 + p3}\end{aligned}\tag{36}$$

## Analytic Damage: Hobler Model

The damage distribution is calculated using [Eq. 35](#) and [Eq. 11, p. 63](#). The primary and lateral distribution functions are taken from the literature [5]. The primary function consists of a Gaussian function and an exponential tail, joined continuously with continuous first derivatives. The distribution is normalized. The normalization factors are  $c_1$  and  $c_2$ , and  $N_{\text{vac}}$  is the number of Frenkel defects per ion.

Three types of primary function are distinguished:

- Type 0: A simple Gaussian distribution with the primary range  $R_p$  and the standard deviation  $\sigma$ :

$$f_p(x) = N_{\text{vac}} c_1 \exp\left(-\frac{(x - R_p)^2}{2\sigma^2}\right)\tag{37}$$

- Type 1: For light ion species:

$$f_p(x) = \begin{cases} N_{\text{vac}} c_1 \exp\left(\frac{x}{l}\right), & x \leq x_0 \\ N_{\text{vac}} c_1 \exp\left(-\frac{(x - R_p)^2}{2\sigma^2}\right), & x > x_0 \end{cases}\tag{38}$$

where  $l$  is the decay length of the exponential function. The joining point  $x_0$  is calculated by:

$$x_0 = R_p - \frac{\sigma^2}{l}\tag{39}$$

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- Type 2: For heavier ions, the exponential tail is directed towards the bulk:

$$f_p(x) = \begin{cases} N_{\text{vac}} c_2 \exp\left(-\frac{(x - R_p)^2}{2\sigma^2}\right), & x \leq x_0 \\ N_{\text{vac}} c_1 \exp\left(\frac{x}{l}\right), & x > x_0 \end{cases} \quad (40)$$

In this model, four parameters  $R_p$ ,  $\sigma$ ,  $l$ , and  $N_{\text{vac}}$  are required. These parameters were obtained by MC simulations between 1 keV and 300 keV. If damage calculation is switched on, that is, if:

```
implant species=<c> damage
```

has been set, Sentaurus Process generates these parameters using an internal lookup table, which contains the original data available for antimony, arsenic,  $\text{BF}_2$ , boron, and phosphorus in silicon.

**NOTE** For some other species, the parameters of these original species are used that are closest with respect to the atomic number in the periodic table of elements. Nitrogen uses the boron parameters. Silicon and aluminum use the phosphorus parameters. Germanium and gallium use the arsenic parameters, and indium uses the antimony parameters. Damage calculation is automatically switched off for any other species.

The Type 0 primary function is used for boron at energies  $E < 20$  keV, phosphorus at  $E < 55$  keV, and arsenic at  $E > 170$  keV. The Type 1 primary function is applied to boron and phosphorus elsewhere, and the Type 2 primary function is applied to arsenic at energies below 170 keV and antimony at all energies.

The lateral distribution is modeled using [Eq. 35, p. 70](#). The lateral parameters ( $p_1, \dots, p_5$ ) are provided in the internal lookup table.

An alternative to the internal lookup table is to load a table file similar to the implantation tables using `dam.table`:

```
implant species=<c> <material> dam.table=<c>
```

This overwrites the internal lookup table for the abovementioned species using the parameters from the table instead. In addition, it enables damage calculation for species other than the original ones.

## Datasets

Several datasets store the as-implanted profile and the implantation damage. Point-defect profiles are created at the end of the implantation step. Datasets with the ending \_Implant contain profiles generated during subsequent implantation steps. These datasets are deleted at the beginning of the next diffusion step.

**Table 6** Datasets used in analytic implantation

Dataset	Description
Damage	Accumulative damage (damage history). At the end of an implantation step, the Damage_LastImp concentration is added to Damage using DFactor. The diffuse command deletes this dataset.
Damage_LastImp	Damage created during the last implantation step. This dataset is deleted at the end of the implantation step.
<dopant>	Accumulative density of the dopant concentration. At the end of an implantation step, the <dopant>_LastImp concentration is added to <dopant>.
<dopant>_Implant	Accumulative density of the dopant concentration. At the end of an implantation step, the <dopant>_LastImp concentration is added to <dopant>_Implant. The diffuse command deletes this dataset.
<dopant>_LastImp	As-implanted dopant concentration that contains the profile generated during the last implantation step. This dataset is deleted at the end of the implantation step.
Int_Implant	Accumulative interstitial profile updated at the end of an implantation step.
Int<component>_Implant	Accumulative interstitial profiles in multicomponent material with DistinctDefects set to true, where <component> is the component of the composition of the material. For example, in SiC, interstitial profiles include IntSilicon_Implant and IntCarbon_Implant.
Vac_Implant	Accumulative vacancy profile updated at the end of an implantation step.
Vac<component>_Implant	Accumulative vacancy profiles in multicomponent material with DistinctDefects set to true, where <component> is the component of the composition of the material. For example, in SiC, vacancy profiles include VacSilicon_Implant and VacCarbon_Implant.

## Implantation Tables

The implantation tables are located at `$SPHOME/Implib/`.

### Default Tables

The `Default` directory contains tables extracted from MC simulations with Crystal-TRIM [6], which are tabulated in Dios format. Data is available for arsenic, antimony,  $\text{BF}_2$ , boron, phosphorus, indium, and germanium in silicon, polysilicon, oxide, and nitride.

The default value for `tables` is `Default`, and the command:

```
implant tables= Default
```

is equivalent to the (default) initialization of *all* species and models at the beginning of each Sentaurus Process run.

These tables provide moments that can be used with all implantation models including dual Pearson. For silicon, dual-Pearson moments are available that depend on energy, tilt, dose, and cap-layer thickness. For polysilicon, oxide, and nitride, single-Pearson moments are available that depend on energy and tilt only.

The tables cover different energy ranges. The tilt angles range from  $0^\circ$  to  $60^\circ$ , and the oxide thickness ranges from 0 nm to 100 nm. There are tables for low, medium, and high doses for all species except germanium where only one table for a medium to high dose is available. Sentaurus Process selects the correct table depending on the implantation dose. These tables constitute most of the default tables used in Sentaurus Process.

This `implant` command not only selects the tables from the `Default` directory for arsenic, antimony,  $\text{BF}_2$ , boron, phosphorus, indium, and germanium in silicon, polysilicon, oxide, and nitride, but also selects the tables from the `Taurus` directory for carbon, fluorine, and germanium in silicon, polysilicon, oxide, and nitride (see [Table 7 on page 75](#)). For all other species and materials, the respective Dios tables are used.

**NOTE** Outside the specified range, the `Default` implantation tables may revert to the `Dios` tables. Therefore, near the boundaries of the `Default` implantation tables, inconsistent results may occur.

Table 7 Default tables

Species	Table file	Energy range [keV]
Antimony	<material>Sb_1e12-5e13.tab <material>Sb_1e13-5e14.tab <material>Sb_2e14-1e16.tab	1.5–600
Arsenic	<material>As_1e12-5e13.tab <material>As_1e13-8e14.tab <material>As_2e14-6e15.tab	0.5–400
BF <sub>2</sub>	<material>BF2_1e12-5e13.tab <material>BF2_1e13-8e14.tab <material>BF2_2e14-6e15.tab	0.5–400
Boron	<material>B_1e12-4e13.tab <material>B_1e13-6e14.tab <material>B_16e13-8e15.tab	0.2–517 (silicon) 0.2–480 (other materials)
Carbon	carbon_in_<material>_standard	0.2–400
Fluorine	fluorine_in_<material>_standard	0.2–400
Germanium	germanium_in_<material>_2007	0.6–800
Indium	<material>In_1e12-4e13.tab <material>In_1e13-6e14.tab <material>In_16e13-8e15.tab	1–400
Nitrogen	nitrogen_in_<material>_standard	0.2–400
Phosphorus	<material>P_1e12-4e13.tab <material>P_1e13-6e14.tab <material>P_16e13-8e15.tab	0.3–400 0.12–3000

## Dios Tables

The `Dios` directory contains the tables used by default in Dios. These implantation tables can be made the default for *all* species in *all* materials in Sentaurus Process using:

```
implant tables= Dios
```

The following command changes all implantation specifications for the species boron from the default to the Dios implantation tables and models:

```
implant species= Boron tables= Dios
```

For arsenic, antimony, phosphorus, indium, germanium, gallium, nitrogen, and aluminum, the data in these tables are taken from the literature [7]. The values for boron are obtained from simulations with the 1D process simulator TESIM [8]. The values for energies  $\geq 1$  MeV are taken from the literature [2]. These tables provide moments that can be used with the Gaussian and Pearson implantation models.

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## Tasch Tables

The Tasch directory contains the University of Texas implantation tables for boron, BF<sub>2</sub>, phosphorus, and arsenic in silicon [9]. For all other materials and species, single-Pearson tables are available. The tables can be selected to be the default using:

```
implant tables= Tasch
```

The tables cover different energy ranges. The boron table `ibout1.s3` contains cap layer-dependent implantation moments valid for thicknesses between 1.5–40 nm. The moments in all other tables are cap layer independent.

Table 8 Tasch tables

Species	Table file	Energy range [keV]
Arsenic	<code>iasut0.s3</code>	7–180
BF <sub>2</sub>	<code>ibfut0.s3</code>	0.5–65
Boron	<code>ibout0.s3</code>	0.5–80
	<code>ibout1.s3</code>	15–80
Phosphorus	<code>iphut0.s3</code>	15–180

The valid range for the tilt is 0° to 10° and, for the rotation, the range is 0° to 45°. These tables provide data to be used with all implantation models.

The single-Pearson tables provide only energy-dependent data covering the range between 10 keV and 1000 keV.

## Taurus Tables

The Taurus directory contains the Taurus Process implantation tables for boron, BF<sub>2</sub>, phosphorus, fluorine, carbon, nitrogen, germanium, indium, antimony, and arsenic. The tables contain calibrated data from sub-keV to above 10 MeV. The calibration was performed using both SIMS data and Taurus MC calculations [10]. This means that Sentaurus Process uses the same moment tables as the Taurus Process implantation library in TSUPREM-4.

To select these tables as the default, use:

```
implant tables= Taurus [data.suf=<c>] [dam.suf=<c>]
```

The file names for Taurus tables are conventionally named:

- `<ion>_in_<material>_<suffix>` for implantation data.
- `<ion>_damage_in_<material>_<suffix>` for damage data.

The default suffix is standard for both implantation data and damage data. You can use the optional arguments `data.suf` and `dam.suf` to change the default suffix for implantation data and damage data, respectively. By using different suffices, different tables for the same species–material combination can coexist in the same directory.

In addition, if `tables=Taurus`, several models are switched on that are not used by default:

- Beam dose control: `beam.dose` (see [Specifying Implantation Parameters on page 54](#))
- Proportional range scaling: `range.sh` (see [Multilayer Implantations on page 84](#))
- Effective channeling suppression: `eff.channeling.suppress` (see [Screening \(Cap\) Layer-Dependent Moments on page 68](#))
- Profile reshaping: `profile.reshaping` (see [Profile Reshaping on page 99](#))
- Preamorphization implantation: `pai` (see [Preamorphization Implantation \(PAI\) Model on page 95](#))

**NOTE** This does not give the same results as `tables=TSuprem4`; however, the results are similar.

## TSUPREM-4 Native Implantation Tables

The `TSuprem4` directory contains the TSUPREM-4 native implantation tables (`s4imp0.ts4`) for antimony, arsenic,  $\text{BF}_2$ , boron, fluorine, indium, and phosphorus. These tables contain the original implantation moments of TSUPREM-4.

To select these tables as the default, use:

```
implant [species=<c>] tables= TSuprem4 [ts4.prefix=<c>]
```

If `species` is specified, TSUPREM-4 native implantation tables are applied to this particular species only. If `species` is not specified, implantation tables are applied to all species supported by TSUPREM-4.

The name of the TSUPREM-4 native implantation table conventionally uses the species name or the species name with a prefix. Eight different implantation tables in silicon are distinguished by a prefix. For example, `chboron` (which means channeling boron) is one of the boron implantation tables in silicon.

The `ts4.prefix` argument takes one of the following values: `default`, `none`, `le`, `ch`, `dual`, `ut`, `tr`, or `scr`:

- `ts4.prefix=default`  
This is the default. It selects the TSUPREM-4 default implantation tables, that is, `antimony`, `fluorine`, `chboron`, `dual.ars`, `dual.pho`, `dual.bf2`, and `tr.indium` for antimony, fluorine, boron, arsenic, phosphorus,  $\text{BF}_2$ , and indium, respectively.

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- `ts4.prefix=none`  
If this is used, no prefix is added. Therefore, the TSUPREM-4 implantation tables (antimony, boron, and so on) are used for antimony, boron, and so on, respectively. If the corresponding table for a species in a material is not available, the default table is used.
- `ts4.prefix=le` or `ts4.prefix=ch`  
If either is used, then `le<species>` or `ch<species>` tables are selected, for example, `leboron` or `chboron` for boron implantation. If the corresponding table for a species in a material is not available, the default table is used.
- `ts4.prefix=dual, ut, tr, or scr`  
If any of these values are used, then `<prefix>.<species>` tables are selected, for example, `dual.boron`, `ut.boron`, `tr.boron`, and `scr.boron` for boron implantation. If the corresponding table for a species in a material is not available, the default table is used.

You also can use your own TSUPREM-4 native-formatted implantation tables using the following command:

```
implant species=<c> <material> imp.table=<c> ts4.species=<c> ts4.material=<c>
```

where:

- `imp.table` specifies the file name (it must include the extension `.ts4`) that contains implantation moment tables in TSUPREM-4 format, for example, `mys4imp0.ts4`. If the file is in the same directory where Sentaurus Process is running, only the name of the file is needed for `imp.table`; otherwise, the full path is required.
- `ts4.species` specifies the TSUPREM-4 table name for the dopant, which is one of the predefined impurity names in the implantation data file. For example, in the standard `s4imp0`, the valid names for boron implantation are `boron`, `leboron`, `chboron`, `ut.boron`, `tr.boron`, and `scr.boron`.
- `ts4.material` specifies the material name used in TSUPREM-4, which is one of the predefined material names in the implantation data file. For example, in the standard `s4imp0`, the material names include `silicon`, `polysilicon`, `oxide`, and `nitride`.

If not specified, `ts4.species` and `ts4.material` default, respectively, to the species name (for example, `Boron`) and the material name (for example, `Silicon`) used in Sentaurus Process.

**NOTE** Ensure that these names match *exactly* the names in the TSUPREM-4 implantation data file. While these names are case insensitive, they cannot be abbreviated. For example, `ts4.material=Polysilicon` will work, but `ts4.material=poly` will generate an error.

---

## Implantation Table Formats

Sentaurus Process handles different table formats and automatically recognizes the format of an implantation table from the file extension.

### Single-Pearson Table Format: <file>.sp

This is the simplest table format that can be used by Sentaurus Process. It contains energy-dependent entries for the moments to be used with the single-Pearson or Gaussian model.

**NOTE** These tables cannot be used with the dual-Pearson model.

The format of the table entries is:

```
*  
energy rp stdev gamma beta lat.stdev
```

There is no dependency of the moments on dose, tilt, rotation, or cap-layer thickness. Lines with an asterisk in the first column are treated as comment lines. Missing or incomplete blocks are not read properly when the file is parsed.

### SUPREM-III Table Format: <file>.s3

This format allows for the handling of dual-Pearson moments that depend on energy, dose, tilt, rotation, and cap-layer thickness. A SUPREM-III implantation table consists of two sections: one for the primary moments and one for the lateral moments. Both sections start with a header, which contains the parameter range covered by the table.

The header is organized as follows:

```
*Energies:  
NumberOfEnergies energy1 energy2 ...  
*Tilts:  
NumberOfTilts tilt1 tilt2 ...  
*Rotations:  
NumberOfRotations rotation1 rotation2 ...  
*Doses:  
NumberOfDoses dose1 dose2 ...  
*Thickness:  
NumberOfThickness thickness1 thickness2 ...
```

**NOTE** The order of these entries must not be changed.

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Lines with an asterisk in the first column are treated as comment lines. A table entry for a particular combination of lookup parameters has the format:

```
*  
rp stdev gamma beta rp2 stdev2 gamma2 beta2 ratio1  
rp stdev gamma beta rp2 stdev2 gamma2 beta2 ratio2  
...  
rp stdev gamma beta rp2 stdev2 gamma2 beta2 ratio<NumberOfDoses>
```

Each line contains eight dual-Pearson moments and the ratio as defined in [Eq. 30, p. 68](#). The entries are ordered increasingly with respect to cap-layer thickness, energy, tilt, and rotation.

**NOTE** There is no automatic check of the order of table entries.

The tables are for one species/material combination only. The cap-layer thickness, `rp`, `rp2`, `stdev`, and `stdev2` must be given in micrometers and the angles, in degrees. The energy values must be specified in keV. No units must be specified in the tables.

The lateral part is organized in the same way. Corresponding to the header information, the entries are ordered in the same manner as in the primary part. Each entry has the format:

```
*  
<void> lstdev lv lstdev2 lv2
```

The first item is void and can be used for information purposes. The parameters are used in [Eq. 33, p. 70](#) to calculate the depth-dependent lateral standard deviation. The unit for `lstdev` and `lstdev2` is micrometer, but `lv` and `lv2` are unitless.

### Dios Table Format: <file>.tab

The Dios table format for implantation data files allows for dependencies on energy, dose, tilt, rotation, and the cap-layer thickness. It provides the primary moments for all implantation models including the dual-Pearson model. Parameters for depth-dependent lateral straggling are available as well. The format of the table entries is:

```
# Look up parameters  
material species thickness rotation tilt energy NumberOfFunctions  
NumberOfDoses  
# Primary moments  
rp stdev <void> gamma beta lexp <void>  
rp2 stdev2 <void> gamma2 beta2 lexp2 <void>  
# Channeling table  
dose ChannelingDose  
dose ChannelingDose  
...  
# Lateral straggling  
p1 p2 p3 p4 p5
```

Lines starting with a hash (#) character in the first column are treated as comment lines. Missing or incomplete blocks are not read properly when the file is parsed.

The first block contains entries for the material and species names, the cap-layer thickness, the rotation angle, the tilt angle, and the energy. The `NumberOfFunctions` defines the number of components of the primary distribution function. A maximum of two functions are allowed. `NumberOfDoses` defines the number of entries in the channeling table. Each entry consists of a dose and the corresponding channeling dose. All doses are expected to be positive.

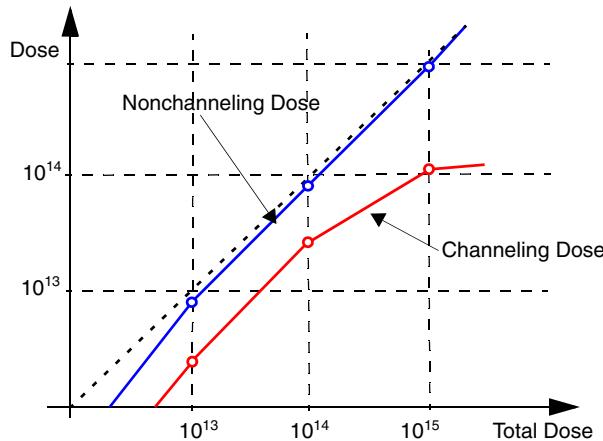


Figure 13 Piecewise linear nonchanneling dose and channeling dose for a dual-Pearson profile as represented in default channeling table

The ratio of the amorphous part and the channeling part in Eq. 30, p. 68 is calculated from the channeling table using:

$$\text{ratio} = 1 - \frac{\text{ChannelingDose}}{\text{dose}} \quad (41)$$

where the value for `ChannelingDose` is interpolated linearly using the value of the implantation dose.

The second block contains the moments for all the components of the primary distribution function. Parameters, which by definition do not exist for the function the set describes, are ignored.

**NOTE** Some entries are always ignored since they are not used in the implantation models of Sentaurus Process. For example, the last moment entry (<void>) is always disregarded.

The third block contains the channeling table ordered with increasing dose, and the fourth block contains parameters for the depth-dependent lateral straggling.

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**NOTE** The entries must be increasingly ordered with respect to the cap-layer thickness, rotation, tilt, and energy, so that the values for various energies (but the same other three parameters) follow each other. All data entries for the same material–dopant combination should follow each other with no interruption by entries for another material–dopant combination. The cap-layer thickness, `rp`, `rp2`, `stdev`, and `stdev2` should be given in micrometers and the angles, in degrees. The energy values must be specified in keV. No units must be specified in the tables.

#### Damage Table Format: <file>.dam

The damage tables for the Hobler damage model are similar to the Dios table format, which allows for dependencies on energy, tilt, and rotation. The Hobler damage model table provides the primary moments for the damage model. Moments for depth-dependent lateral straggling are available as well. The format of the table entries is:

```
# Look up parameters
material species rotation tilt energy
# Primary moments
rp stdev decay nvac type
# Lateral straggling
p1 p2 p3 p4 p5
```

The syntax is the same as for the Dios table format. The item `decay` refers to the parameter  $l$ , and the item `nvac` refers to the parameter  $N_{vac}$  in [Analytic Damage: Hobler Model on page 71](#). The item `type` refers to the type of Hobler model.

#### Taurus Table Format: <file>

The Taurus table format, which is the most general table format used in Sentaurus Process, handles data for all implantation and damage models. Implantation tables in the Taurus format have no file extension, that is, an implantation table without a file extension is considered to have the Taurus table format.

It contains a file header and a block of numeric data. The file header consists of a list of names of the implantation conditions. The names must be lowercase only. The following names are recognized:

```
energy tilt rotation dose screen temperature current
```

The sequence of these names can be arbitrary. Some of these names can be omitted. The following units must be used for the implantation conditions:

```
energy, [keV]
tilt, [degrees]
rotation, [degrees]
```

```
dose, [cm-2]  
screen, [um]  
temperature, [K]  
current, [mA/cm2]
```

The numeric data consists of an arbitrary number of lines that form the lookup tables for implantation conditions and implantation moments. Each line should contain a list of numeric values for the implantation conditions followed by the implantation moments. The numeric values must be separated by whitespace.

The number of numeric values must be the same on each line. There should be at least  $n+4$  values per line for a Gaussian profile,  $n+6$  values per line for a Pearson profile, and  $n+13$  values per line for a dual-Pearson profile, where  $n$  is the number of the implantation conditions specified in the file header.

The sequence of implantation conditions must correspond exactly to the sequence of implantation condition names in the file header. The sequence of the implantation moments in one line is fixed as follows:

Gaussian: rp stdev lat.stdev lat.slope

Pearson: gamma beta

Dual Pearson: rp2 stdev2 lat.stdev2 lat.slope2 gamma2 beta2 ratio

Any line that starts with a double slash (//) is considered a comment and is omitted. Always put the double slash at the first position in the line.

If the requested set of implantation conditions does not have an exact match in the lookup table, a multidimensional linear interpolation is used. If a requested implantation condition extends beyond the range of the lookup table, the closest value from the lookup table is used.

If the lookup table contains several lines with identical sets of implantation conditions, only the last set is used, and all the previous lines are discarded.

If a table contains data for the Hobler damage model, the following sequence of moments is used:

```
rp stdev lat.stdev lat.slope gamma beta decay nvac
```

### 3: Ion Implantation

#### Analytic Implantation

## Multilayer Implantations

Point-response functions are valid only for a single-material layer. For multiple layers of different materials, the point-response functions must be combined in a way that corrects the effect of different stopping powers in the covering layers. This must be performed for each lateral interval taking into account the local layer sequence, parallel to the ion beam. Two algorithms are available in Sentaurus Process:

- Numerical range scaling (NRS) [11]
- Dose-matching [9]

Both algorithms calculate a shift  $\delta_i$  applied to the primary point-response function. Sentaurus Process also provides an option no, which switches off the matching. In this case,  $\delta_i$  is set to zero in all layers.

The matching algorithm can be selected globally using the command:

```
adbSet ImplantData MatchControl {range | dose | no}
```

The default value of MatchControl is range.

In addition, you can select locally the matching algorithm using match in each implant command:

```
implant <species> match= range | dose | no
```

The locally selected algorithm overwrites the one globally set in the Parameter Database (PDB).

The NRS algorithm accounts for the different stopping powers in different materials using the ratio of the projected ranges of the materials.

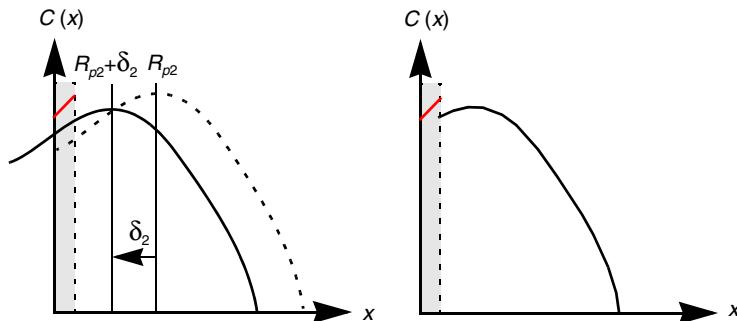


Figure 14 NRS algorithm: (left) the point-response function in the second material is shifted and rescaled due to existence of a layer with different stopping power (shaded region), and (right) the new profile is combined from the point response in the first layer and the shifted point response in the second layer

The shift in the  $i$ -th layer is calculated according to:

$$\delta_i = \sum_{j=1}^{j < i} t_j \left( 1 - \frac{R_{pi}}{R_{pj}} \right) \quad (42)$$

where  $t_j = d_j - d_{j-1}$  represents the thickness of the  $j$ -th layer. The profiles are matched according to:

$$C(x) = \begin{cases} f_{p1}(x) & \text{for } 0 < x < d_1 \\ \alpha_i \cdot f_{p1}(x - \delta_i) & \text{for } d_{i-1} < x < d_i \end{cases} \quad (43)$$

where  $\alpha_i$  is a rescaling factor that satisfies the normalization condition. The point-response function in the first layer is always used without a shift.

The *proportional range shift model* is used to shift the channeling portion of the implantation profile independent of the amorphous part. To calculate the shift of the channeling part, the shift of the amorphous part is scaled by the ratio of the channeling range and the amorphous range:

$$\delta_{i, \text{tail}} = \delta_{i, \text{head}} \frac{R_{pi, \text{tail}}}{R_{pi, \text{head}}} \quad (44)$$

The proportional range scaling can be switched on with:

```
implant <species> range.sh
```

The default setting for this model is off. In the Taurus or TSUPREM-4 mode, the range scaling is switched on.

The dose-matching algorithm can be selected with `dose`. The shift  $\delta_i$  is calculated according to the dose accumulated in the above layers:

$$\delta_i = d_i - d_{\text{eff}}$$

$$D_{\text{sofar}} = \int_0^{d_{\text{eff}}} f_p(x) dx \quad (45)$$

where  $d_i$  is the position of the top of the  $i$ -th layer. The dose  $D_{\text{sofar}}$  is the integral over the primary point-response function.

## Lateral Integration

### Local Layer Structure in Two Dimensions

Local 1D layer structures are defined for a set of lateral intervals. These lateral intervals are chosen perpendicular to the projection of the ion beam into the simulation plane as shown in Figure 15.

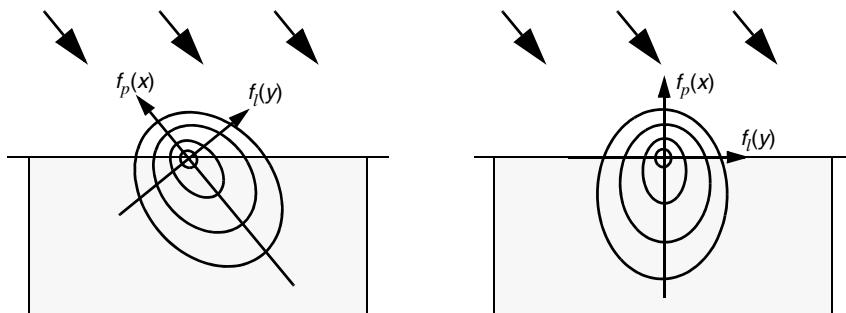


Figure 15 (Left) Beam projection mode and (right) wafer normal mode for analytic implantation

The width of the lateral intervals is controlled by several parameters set in the parameter database. The default values can be changed using:

```
pdbSet ImplantData LateralGridSpacing <n>
pdbSet ImplantData VerticalGridSpacing <n>
```

Starting from an initial grid, the intervals are bisected until a certain limit is reached. This limit is set by `LateralGridSpacing`, which has the default value of  $0.01 \mu\text{m}$ . Then, the intervals are bisected again until a certain vertical limit is reached. This limit is set by `VerticalGridSpacing` with the default value of  $0.01 \mu\text{m}$ .

The lateral integration is limited to a certain range of intervals to the left and right of a mesh node. This integration range depends on the maximum lateral standard deviation applied to the structure.

Control over the lateral integration is possible by setting the number of lateral standard deviations used to set the integration range:

$$C(x, y) = \int_{y - N\sigma_{l, \max}}^{y + N\sigma_{l, \max}} f_p(x)f_l(x, y')dy' \quad (46)$$

The value of  $N$  can be set using:

```
pdbSet ImplantData NumLateralStdev <n>
```

The default value is 5, which means that the total lateral integration width is  $10 \sigma_{l, \text{max}}$ .

In three dimensions, the integration is performed over a square grid in the plane perpendicular to the ion beam. The grid is centered about a mesh node. It has a fixed size and resolution. The size is controlled by the parameter:

```
pdbSet ImplantData NumLateralStdev3D <n>
```

having the same meaning as the corresponding 2D parameter. The default value is 3.5. Each interval is subdivided by a certain number of grid points. The subdivision can be set using:

```
pdbSet ImplantData NumGridPoints3D <n>
```

so that the total number of grid points is  $(2 \cdot \text{NumLateralStdev3D} \cdot \text{NumGridPoints3D})^2$ .

The default value for `NumGridPoints3D` is 4. Therefore, the total number of grid points is 784. The size of the integration grid is the parameter that limits the time performance of analytic implantation in three dimensions.

**NOTE** The default value of `NumGridPoints3D` is a trade-off between speed and accuracy. Under certain implantation conditions, especially at high energy, the profiles may exhibit stepped, striped, or noisy behavior. In such cases, you may increase `NumGridPoints3D` to as much as 20.

The lateral intervals are expanded by a certain amount over the left and right boundaries of the 2D device to ensure flat profiles on the left and right sides. This extension depends on the implantation tilt and the maximum lateral standard deviation. The maximum extension can be controlled from the parameter database. The value can be changed using:

```
pdbSet ImplantData MaxLateralExtension <n>
```

The default is set to  $1.5 \mu\text{m}$ . A similar extension is applied in three dimensions.

## Primary Direction and Scaling

The interpretation of the range and the lateral range parameters depends on the value of `primary`:

```
implant <species> primary= beam | wafer
```

### 3: Ion Implantation

#### Analytic Implantation

The option `beam` switches to the beam projection mode. In this case, the primary moments are applied along the projection of the ion beam on to the simulation plane, and the lateral integration is performed perpendicular to the projection of the ion beam. This is the default mode in Sentaurus Process.

The option `wafer` switches to the wafer normal mode. Here, the primary distribution function and the moments are interpreted orthogonally to the wafer surface.

An implantation table can be declared to be angle dependent or angle independent using:

```
implant species=<c> angle.dependent
```

Tilt-dependent and rotation-dependent data values extracted from SIMS measurements or user-specified range parameters are assumed to be angle dependent. On the other hand, theoretical range parameters, such as those calculated by Lindhard, Scharff, and Schiøtt (LSS) theory, are assumed to be angle independent.

For the same pair of `tilt` and `rotation` parameters, different projected tilt angles can be observed in the 2D simulation plane. This angle is called `tilt2D` and depends on both `rotation` and `slice.angle`. Profiles in quasi-1D parts of the structure away from mask edges depend on the choice of `slice.angle`. Exactly the same 1D profiles can be observed only for symmetric primary distribution functions like the ones used in the Gaussian model and only if the primary and lateral standard deviations have the same value.

To ensure, at least approximately, that the same depth profiles are obtained for different rotation angles and for different dimensions, the range parameters for the primary distribution function are scaled depending on `tilt` (for one dimension and three dimensions) or `tilt2D` (for two dimensions). For example, the projected range  $R_p'$  is scaled as follows:

$$R'_p = R_p \cdot s_r \quad (47)$$

For tilt implantations, the integrated dopant profile depends not only on the primary range parameters ( $R_p$ ,  $\sigma_p$ , and so on), but also on the lateral straggling ( $\sigma_l$ ). To ensure that the same depth profiles are obtained approximately for different rotation angles and for different dimensions, the primary standard deviation is scaled as follows:

$$\sigma'_p = \sqrt{s_r^2 \cdot \sigma_p^2 + (1 - s_r^2) \cdot \sigma_l^2} \quad (48)$$

Note that if the ratio  $\sigma_l/\sigma_p$  is too large, the scaling of the primary standard deviation may not be possible. In such a case, Sentaurus Process issues a warning message and continues by assuming  $\sigma'_p = \sigma_p$ .

The scaling factor  $s_r$ , which is used to scale  $R_p$  and  $\sigma_p$ , is selected with respect to the values of `primary` and `angle.dependent`, as shown in [Table 9 on page 89](#).

Table 9 Scaling factor for the primary range

Dimension	primary	!angle.dependent	angle.dependent
One	wafer	$s_r = \cos(\text{tilt})$	$s_r = 1$
	beam	$s_r = \cos(\text{tilt})$	$s_r = 1$
Two	wafer	$s_r = \cos(\text{tilt})$	$s_r = 1$
	beam	$s_r = \frac{\cos(\text{tilt})}{\cos(\text{tilt2D})}$	$s_r = \frac{1}{\cos(\text{tilt2D})}$
Three	wafer	$s_r = \cos(\text{tilt})$	$s_r = 1$
	beam	$s_r = 1$	$s_r = \frac{1}{\cos(\text{tilt})}$

## Point-Response Interface

The point-response interface allows the use of externally generated point responses in analytic implantation. As an alternative to using implantation tables, it replaces the moment-based point-response distributions. Only 1D primary distributions can be loaded with Sentaurus Process.

To use the point-response interface, change the implantation model to `point.response`, for example:

```
implant species=<c> <material> point.response file=<c> y.position=<n>
```

To revert to the moment-based point-response distribution, switch to one of the analytic functions, for example, switch to the dual-Pearson model for boron in silicon:

```
implant species= Boron Silicon dualpearson
```

The default table setting can be used again since it has not been overwritten by `point.response`.

The external primary distribution function and the damage are read from a `.plx` file. A separate file can be selected for each species–material combination with the `file` argument and the above command.

The 1D MC implantation run is started to generate the data if the file is not found. This run is fully automated. The 1D layer structure for this run consists of an oxide layer on top and a layer of the specified material. The thickness of the oxide layer is chosen as the total effective overlayer thickness at some point of reference at the gas surface of the structure. The position of this point at the y-axis is specified with the `y.position` argument.

### 3: Ion Implantation

#### Analytic Implantation

The integration routine treats the data as a continuous set to be used in the material as specified. In the convolution integral computation, the zero of the x-axis is locally matched to the surface of the structure.

The initial damage for the MC implantation is taken from the damage already present in the device along a line starting from the surface at the `y.position` normal to the wafer surface.

The external profiles are interpreted as being normal to the wafer surface. Therefore, the direction of the primary distribution must change from `beam` to `wafer` (see [Primary Direction and Scaling on page 87](#)). In addition, the multilayer matching method must be set to dose-matching (see [Multilayer Implantations on page 84](#)), that is:

```
implant <species> primary= wafer match= dose
```

The value for the primary range  $R_p$  is taken from the implantation table if `match=range`.

---

## Implantation Damage and Point-Defect Calculation

Analytic implantation can generate damage profiles that are stored in the dataset `Damage`, and interstitial and vacancy profiles that are stored in the datasets `Int_Implant` and `Vac_Implant`, respectively.

### Implantation Damage

The damage to the crystal is calculated on the basis of analytic damage models. Sentaurus Process calculates the damage using the model by Hobler and Selberherr [1]. Damage calculation for a species in a material can be switched on using `damage`:

```
implant species=<c> <material> damage
```

A damage profile is calculated if `damage` is set and the moments are found in the internal lookup table. Sentaurus Process can use the moments provided by [1] as described in [Analytic Damage: Hobler Model on page 71](#). At the end of an implantation step, the damage for this step (`Damage_LastImp`) is added to the `Damage` profile (damage history) using:

$$\text{Damage} += \text{DFactor} \cdot \text{Damage}_\text{LastImp} \quad (49)$$

where `+=` indicates that the total damage is the sum of the new damage and the existing damage.

The default value for `DFactor` is 1, which can be changed in the `implant` command or in the parameter database:

```
implant <species> dfactor=<n>
pdbSetDouble <material> <dopant> DFactor <n>
```

## Point-Defect Calculation: Elemental Materials

The interstitial and vacancy profiles are calculated in a postprocessing step at the end of the `implant` command. The model used to calculate point defects is selected using `defect.model`:

```
implant <species>
defect.model= effective.plus.n | frenkel.pair | plus.one | userdefined
```

### The `effective.plus.n` Model

The `effective.plus.n` option selects the ‘+n’ model to calculate dynamically an `NFactor` using an energy-dependent and a dose-dependent fitting formula after Hobler and Moroz [12]. The `NFactor` replaces the `IFactor` in Eq. 52. The ‘+n’ model provides an improved way to calculate the interstitial profile for heavy ions and low implantation doses. Under these implantation conditions, the `NFactor` can significantly deviate from 1 [12].

### The `frenkel.pair` Model

The `frenkel.pair` option selects the Frenkel pair model with which the interstitial and vacancy profiles are calculated from the damage and dopant profiles resulting from the last implantation step:

$$\begin{aligned} \text{Int_Implant} &+= \text{FPIFactor} \cdot \text{Damage}_\text{LastImp} + \text{IFactor} \cdot <\text{dopant}>_\text{LastImp} \\ \text{Vac_Implant} &+= \text{FPVFactor} \cdot \text{Damage}_\text{LastImp} \end{aligned} \quad (50)$$

where the `<dopant>_LastImp` term accounts for the extra interstitials coming from substituted dopants. `FPIFactor` and `FPVFactor` can be set in the parameter database and can be overwritten using `fp.ifactor` and `fp.vfactor` in the `implant` command.

If `crit.dose` is defined, the given value of `IFactor` in the ‘+1’ model and the damage model for point defects is taken from:

$$\text{IFactor} = \text{IFactor} \cdot \min \left( 1, \frac{\text{crit.dose}}{\text{dose}} \right) \quad (51)$$

### 3: Ion Implantation

Analytic Implantation

#### The plus.one Model

The `plus.one` option selects the ‘+1’ model to calculate the interstitial and vacancy profiles from the as-implanted profile at a particular implantation step `<dopant>_LastImp`:

$$\begin{aligned} \text{Int\_Implant} &+= \text{IFactor} \cdot <\text{dopant}>_{\text{LastImp}} \\ \text{Vac\_Implant} &+= \text{VFactor} \cdot <\text{dopant}>_{\text{LastImp}} \end{aligned} \quad (52)$$

where `IFactor` and `VFactor` are material-dependent factors that can be set in the parameter database. For example, for boron in silicon, this is performed using:

```
pdbSet Silicon Boron IFactor <n>
```

The internal default values are 1 for `IFactor` and 0 for `VFactor`. This is motivated by a simple lattice site balance argument: for each dopant atom that is assumed after implantation on a lattice site, one free interstitial is produced. The global values for `IFactor` and `VFactor` can be overwritten in the `implant` command:

```
implant <species> <material> ifactor=<n> vfactor=<n>
```

#### The user.defined Model

The `user.defined` option allows you to define your own algorithms to calculate interstitial and vacancy profiles. It is expected that you will define the algorithm in the `UserPointDefectModel` procedure, for example:

```
fproc UserPointDefectModel { Species Name Energy Dose Model IFactor \
    VFactor CDose } {
    ...
}
```

where:

- `Species` is the name of the implanted species.
- `Name` is the name of the dopant.
- `Energy` is the implantation energy.
- `Dose` is the implantation dose.
- `Model` is the implantation model (for example, `tables` or `sentaurus.mc`).
- `IFactor` and `VFactor` are the interstitial and vacancy factors.
- `CDose` is the critical dose.

## Point-Defect Calculation: Multicomponent Materials

In multicomponent materials, such as silicon carbide (SiC), the material is composed of different atom types. When an impurity is implanted into SiC, both silicon and carbon lattice atoms can be displaced, thereby forming silicon interstitials or carbon interstitials, and leaving behind silicon-site or carbon-site vacancies. Instead of classifying them together as interstitials or vacancies, as in silicon, Sentaurus Process provides a mechanism to distinguish different types of interstitial or vacancy.

To generate distinct types of point defect in multicomponent materials, you must switch on the `DistinctDefects` flag, for example:

```
pdbSetBoolean SiliconCarbide DistinctDefects 1
```

By default, this flag is true for SiC but false for other materials. As a result, instead of `Int_Implant` and `vac_Implant`, the generated point-defect datasets in SiC are `IntSilicon_Implant`, `IntCarbon_Implant`, `VacSilicon_Implant`, and `VacCarbon_Implant`.

In this model, the total point-defect concentration is computed in the same way as the elemental material. The implantation parameters `defect.model`, `ifactor`, `fp.ifactor`, and `fp.vfactor` of the `implant` command still work. The parameters `ifactor` and `vfactor` are scaling factors for interstitial profiles and vacancy profiles, respectively, in the `plus.one` model; while `fp.ifactor` and `fp.vfactor` are scaling factors for interstitial profiles and vacancy profiles, respectively, in the `frenkel.pair` model. The same Tcl procedure `CalcPlusNFactor` calculates automatically the `plus` factors for the `effective.plus.n` model.

Then, the individual point-defect concentration is computed by multiplying the total point-defect concentration by the fraction of each component. The fraction of each component is, by default, their stoichiometric weight, but it can be changed in the parameter database with the parameters `IFactor.Fraction` and `VFactor.Fraction`. For example, in SiC:

```
pdbSet SiC Composition Component0 IFactor.Fraction <n>
pdbSet SiC Composition Component1 IFactor.Fraction <n>
pdbSet SiC Composition Component0 VFactor.Fraction <n>
pdbSet SiC Composition Component1 VFactor.Fraction <n>
```

### 3: Ion Implantation

#### Analytic Implantation

## Backscattering Algorithm

During implantation, some particles may be backscattered and lost to the ambient. Analytic implantation accounts for this effect by assuming that a portion of the distribution that protrudes from the structure is backscattered from the surface, resulting in less dose being implanted in the structure.

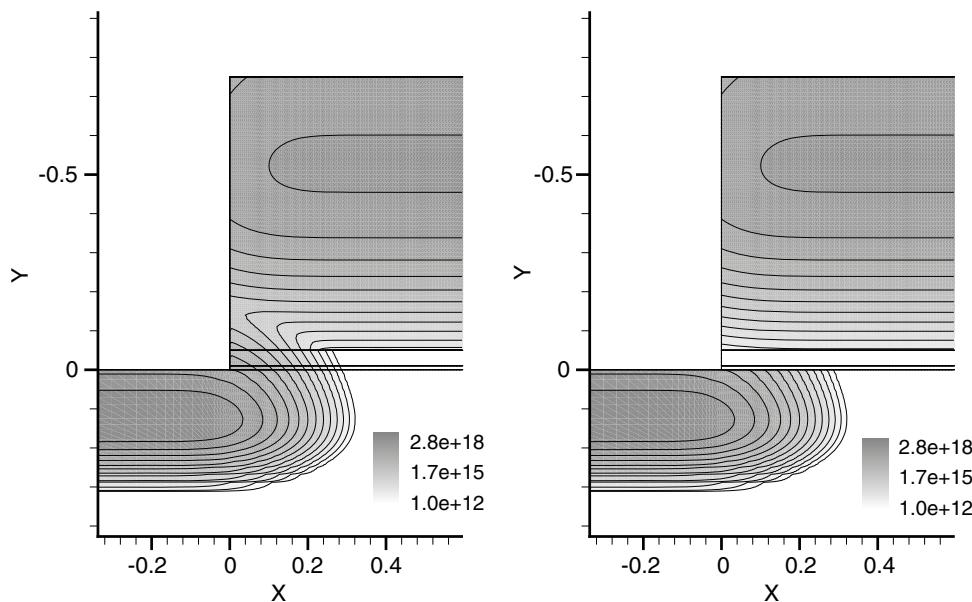
This backscattering model – the TS4 backscattering model – is switched off by default. To switch on the model, either specify `ts4.backscattering` in the `implant` command or use the global switch:

```
pdbSet ImplantData TS4Backscattering 1
```

In addition to the TS4 backscattering model, Sentaurus Process uses an advanced integration algorithm that accounts for particles backscattered from the surface. The lateral integration for a mesh node also is performed over 1D intervals above the surface. The point response is taken from the surface layer. The contributions from backscattered ions make a difference in the profile of vertical mask edges. The mask example in [Figure 16](#) illustrates the difference.

This backscattering algorithm is switched on by default. To switch off the algorithm, use either `!backscattering` in the `implant` command, or the global switch:

```
pdbSet ImplantData Backscattering 0
```



**Figure 16** Boron implantation at a vertical mask edge (*left*) with backscattering and (*right*) without backscattering; tilt angle is  $0^\circ$  and energy is 35 keV

---

## Multiple Implantation Steps

### Preamorphization Implantation (PAI) Model

A structure already has implantation-related damage by the time an implantation is performed. This damage contributes to the suppression of the channeling tail. This applies to a series of implantations performed without intermediate anneals. In this case, an equivalent amorphous thickness is extracted as:

$$t_{i, \text{eqv}} = \frac{1}{\text{PAIThreshold}} \sum_{j=x_i}^{j \leq i} \int \text{Damage} dx \quad (53)$$

where `Damage` denotes the pre-existing implantation damage in terms of Frenkel pairs, and `PAIThreshold` is a normalization parameter that can be specified in the parameter database:

```
pdbSet <material> PAIThreshold <n>
```

This normalization parameter is used for all species in this material, unless you specify the species-specific parameter using the following PDB command:

```
pdbSetDouble <material> <species> PAIThreshold <n>
```

The extracted equivalent amorphous thickness is added to the total amorphous layer thickness. If the implantation table contains screen (cap) layer-dependent data, the total amorphous thickness is used as a parameter to select the implantation moments as described in [Screening \(Cap\) Layer-Dependent Moments on page 68](#). Otherwise, the profile reshaping model and the effective channeling suppression model are used.

The integral over the preamorphizing damage assumes periodic boundary conditions for the structure in two dimensions.

To switch on the PAI model, use:

```
implant <species> energy=<n> dose=<n> pai
```

**NOTE** The PAI model is switched off by default. It is switched on for the Taurus implantation tables.

### ColImplant Model

The fraction of the ions described by the second Pearson function is taken from implantation tables, which have been created for single ion implantation steps. This treatment is acceptable

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#### Analytic Implantation

only for low-dose implantations, which create little crystal damage, but it leads to a severe overestimation of the ion channeling in successive implantations with medium and high doses.

Without a thermal annealing step between several ion implantations, the crystal damage of the first implantations remains present and reduces the ion channeling of the subsequent implantations. The channeling tail is lowered. Besides the PAI model, analytic implantation provides the CoImplant model, which also takes this effect into account. In contrast to the PAI model in which the implantation moments are modified locally for each cutline during the integration, the CoImplant model modifies the channeling ratio globally for each implantation. The CoImplant model is switched on using the command:

```
pdbSetBoolean ImplantData UseCoImplant 1
```

The CoImplant model is switched on by default.

**NOTE** The CoImplant model is active only for the Default implantation tables and does not affect any other implantation tables.

The CoImplant model considers damage produced by analytic or MC implantation steps. The damage information is used in subsequent analytic implantation steps to estimate the channeling ratio.

Using a least-square fit, an equivalent dose  $D^{eq}$  is calculated. This dose is chosen as the dose that would give the same amount of damage in one implantation step (using the present species and implantation conditions) as the pre-existing damage, that is:

$$\int (\text{damage}[D^{eq}(x)] - \text{damage}_{\text{preexist}})^2 dx = \min \quad (54)$$

This is used to calculate the channeling dose  $D_c^{\text{new}}$  from the total channeling dose and the equivalent channeling dose, that is:

$$D_c^{\text{new}} = D_c^{\text{total}} - D_c^{eq} \quad (55)$$

The channeling dose is calculated from the total dose using the differential channeling dose technique (see [Figure 17 on page 97](#)).  $D_c^{\text{total}}$  is the channeling dose corresponding to an implantation of  $D_c^{eq} + D_c^{\text{new}}$  into undamaged silicon.

In [Figure 17](#), due to the creation of damage during implantation, the number of channeling ions increases sublinearly with the total ion dose, and it eventually saturates at very high total doses. The damage from previous implantations is set equivalent to a dose  $D^{eq}$ . The dose of the additional implantation is shifted and, consequently, the gradient  $D_c^{\text{new}}/D^{eq}$  and, therefore, the dual-Pearson ratio are reduced.

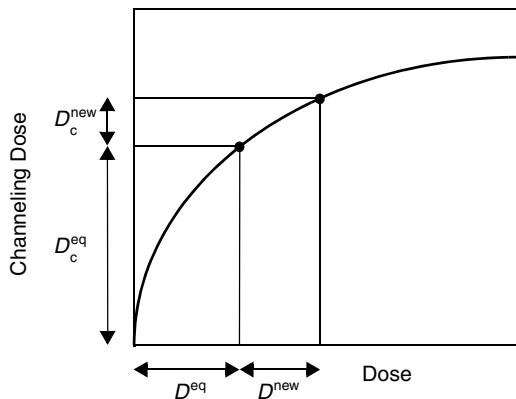


Figure 17 Channeling dose as a function of dose

Both  $D_c^{eq}$  and  $D_c^{total}$  are stored in lookup tables. The channeling dose  $D_c^{new}$  is used to calculate the new ratio for the dual-Pearson model (see [Primary Distribution Functions on page 63](#)).

This simple model is very accurate for mixed species implantations and works best in cases of subsequent implantations with similar energies. The model is only available for the Default implantation mode.

The simplest way to calibrate the strength of de-channeling is given by using the effective damage factor that scales the calculated equivalent dose:

```
 pdbSetDouble ImplantData <species> EffDamFac <factor>
```

The default value is 1. Increased values lead to less channeling; lower values increase the channeling of the species specified.

To calibrate the effective damage factor depending on parameters of the implantation, the following procedure must be overwritten:

```
fproc CI::coimp_dosesofar_calib { species energy dose tilt rotation } {
    switch $species {
        Boron { set cuc <expression_for_Boron> }
        default { set cuc 1.0 }
    }; # end of switch
    return $cuc
}
```

Sometimes, it will be necessary to reset the accumulated damage field internally used by the CoImplant model. This can be achieved using:

```
CI::Reset
```

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To save and load the accumulated damage field, use:

```
CI::Save <filename>
CI::Load <filename>
```

The loaded damage is added to the existing accumulated damage. The accumulated damage produced by any implantation history can be checked with:

```
CI::Get_Damage_pdb Accumulated_Damage
```

This returns a list containing the vector describing the damage in the wafer on a logarithmic depth scale. A zero vector means no damage history is seen by any follow-up table implantation.

For more details about the CoImplant model, see [\[13\]](#).

To choose the PAI or CoImplant model, use the global switch `DamageControl`:

```
pbSet ImplantData DamageControl {Default | CoImplant | PAI}
```

The default value of `DamageControl` is `Default` in which the PAI model is automatically switched on when Taurus tables are used. Whereas, the CoImplant model is chosen when default tables are used. If `DamageControl` is set to `PAI`, the PAI model is active for all subsequent implantations regardless of which tables are used. If `DamageControl` is set to `CoImplant`, the CoImplant model is used for all subsequent implantations (note that the CoImplant model only supports default tables), and PAI is disabled even for Taurus tables.

**NOTE** Both the PAI model and the CoImplant model are designed to take into account the pre-existing damage. However, the PAI model modifies the implantation moments locally, while the CoImplant model modifies the channeling ratio globally. Generally, for a complex structure, the PAI model is more accurate at the expense of a longer computation time.

**NOTE** The CoImplant model is designed to work on the same structure among a sequence of implantation steps. If the structure changes between implantations, erroneous results could occur.

**NOTE** To avoid double-counting the damage effect, when the PAI model is active, the CoImplant model is disabled automatically.

## Profile Reshaping

The profile reshaping model can be switched on using:

```
implant <species> profile.reshaping
```

The model remains inactive for explicitly cap layer-dependent implantation tables.

**NOTE** This model is switched off by default, and it is switched on in the Taurus or TSUPREM-4 mode.

Traditionally, it is believed that the first peak of the implanted profile in monocrystalline silicon is due to random scattering and is described by the first Pearson distribution in the dual-Pearson analytic model. The second peak (or hump) of the implanted distribution is attributed to ion channeling and is described by the second Pearson distribution in the dual Pearson model.

This approach works well for implantations with tilt angles above approximately  $4^\circ$ , where the position and width of the first Pearson distribution do not change as a function of the screen oxide thickness. However, for low tilt implantations (below  $4^\circ$ ), the position and width of the first Pearson distribution changes considerably (up to 50%) with the thickness of the screen oxide.

Typically, for a low-tilt implantation performed into bare silicon, the first Pearson distribution shifts deeper into the substrate and is much wider than for a similar high-tilt implantation. As the screen oxide thickness increases, the projected range and the standard deviation of the first Pearson distribution relax to their respective values at high tilt angles due to reduced channeling. Physically, this means that, for a low-tilt implantation, even the first peak contains a considerable number of channeled ions. To model this effect, it is necessary to reshape both Pearsons in the dual-Pearson model. This profile reshaping complements the reduction in channeling fraction provided by the effective channeling suppression model.

For ions with explicit dependency on the screen oxide thickness in the implantation tables, this change in shape is addressed automatically. Otherwise, a shift is added to the projected range, the standard deviation, and the lateral standard deviation of both Pearson distributions. The shift is given by:

$$\Delta_i = \left( 1 - e^{-\frac{\alpha_i t}{\sigma}} \right) (MH_i - ML_i) \quad (56)$$

where:

- $\Delta_i$  is the shift for moment  $i$ .
- $\alpha_i$  is the shift factor for moment  $i$ .
- $t$  is the cap-layer thickness.

### 3: Ion Implantation

#### Analytic Implantation

- $MH_i$  is the value of moment  $i$  at high tilt value ( $7^\circ$ ).
- $ML_i$  is the value of moment  $i$  at a given low tilt angle.
- For historical reasons,  $\sigma$  is the standard deviation of the first Pearson distribution. However, this normalization quantity can be switched to the projected range using the command:

```
pdbSet ImplantData ProfileReshaping.Rp 1
```

The shift factor parameters of the profile reshaping model can be set in the parameter database, that is:

```
pdbSet <material> <species> RangeFactor  
pdbSet <material> <species> SigmaFactor  
pdbSet <material> <species> ChannelingRangeFactor  
pdbSet <material> <species> ChannelingSigmaFactor
```

The value of `RangeFactor` is used when calculating the shift of the projected range. The value of `SigmaFactor` is used for both the standard deviation and the lateral standard deviation. Setting a shift factor to zero effectively switches off this model for the respective moments. Higher values of the shift factor lead to a faster transition from a low tilt profile to a high tilt profile, with increasing amorphous layer thickness. By default, the shift factors are zero in all materials except silicon.

---

## Germanium-Dependent Analytic Implantation

SiGe material technology is used widely in stress engineering to improve device performance (such as mobility). In addition, the depth of the source/drain junctions in  $Si_{1-x}Ge_x$  can be greatly reduced by increasing the Ge content, which results from, not only the reduced boron diffusion for PMOS source/drain, but also the reduced projected range and channeling in as-implant itself.

Since the average mass of the atomic nucleus of the target is heavier in SiGe than in pure silicon, a scattering angle from a nuclear collision is larger. In addition, SiGe has a larger electronic stopping power than silicon due to the higher electron density. Therefore, similar to the PAI model, the Ge effect on implantation can be modeled by using similar models for profile reshaping and effective channeling suppression.

In this Ge-dependent model, first the equivalent germanium thickness is extracted:

$$t_{Ge, eqv} = \frac{1}{GeThreshold} \int C_{Ge} dx \quad (57)$$

where  $C_{Ge}$  denotes the germanium concentration and GeThreshold is a normalization parameter that can be specified in the parameter database:

```
pdbSet <material> <species> GeThreshold <n>
```

Then, the following formulas are used for the projected range reduction and the standard deviation shift:

$$\Delta R_{P, Ge} = -Ge.RangePreFactor \cdot R_{P, 0} \cdot \left( 1 - \exp\left(-Ge.RangeFactor \cdot \frac{t_{Ge, eqv}}{R_{P, 0}}\right) \right) \quad (58)$$

$$\Delta \sigma_{Ge} = -Ge.SigmaPreFactor \cdot \sigma_{Ge, 0} \cdot \left( 1 - \exp\left(-Ge.SigmaFactor \cdot \frac{t_{Ge, eqv}}{R_{P, 0}}\right) \right)$$

where:

```
Ge.RangePreFactor  
Ge.RangeFactor  
Ge.SigmaPreFactor  
Ge.SigmaFactor
```

can be specified, respectively, in the parameter database as:

```
pdbSet <material> <species> Ge.RangePreFactor <n>  
pdbSet <material> <species> Ge.RangeFactor <n>  
pdbSet <material> <species> Ge.SigmaPreFactor <n>  
pdbSet <material> <species> Ge.SigmaFactor <n>
```

Similar formulas also exist for the channeling projected range and the channeling standard deviation shifts with the parameter names:

```
Ge.ChannelingRangePreFactor  
Ge.ChannelingRangeFactor  
Ge.ChannelingSigmaPreFactor  
Ge.ChannelingSigmaFactor
```

Finally, the following formula is used for effective channeling suppression:

$$r_{Ge} = r_{Ge, 0} \cdot \left( \frac{Ge.Sup.Ratio}{Ge.Sup.Ratio + \frac{t_{Ge, eqv}}{R_{P, 0}}} \right)^{Ge.Sup.Exponent} \quad (59)$$

where Ge.Sup.Ratio and Ge.Sup.Exponent can be specified in the parameter database:

```
pdbSet <material> <species> Ge.Sup.Ratio <n>  
pdbSet <material> <species> Ge.Sup.Exponent <n>
```

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#### Analytic Implantation

---

## Analytic Molecular Implantation

Sentaurus Process allows for the implantation of arbitrary molecular species (such as  $\text{BF}_2$  and  $\text{B}_{10}\text{H}_{14}$ ). The implantation can proceed with or without the implantation tables for the molecular species. If implantation tables are unavailable for the molecular species, an approximate calculation of the dopant distribution is performed, based on the tables for the primary dopant species. Therefore, the only requirement for analytic molecular implantation is that implantation data tables are available for the primary dopant species (such as B, As, or P).

The primary dopant species, for which the profile is calculated, is specified using dataset in the `implant` command:

```
implant species=<c> dataset=<c>
```

To switch on the damage calculation in silicon for analytic molecular implantation, use:

```
implant species=<c> Silicon damage
```

In a molecule, the implantation energy is shared by several atoms according to:

$$E_i = \text{energy} \cdot \frac{M_i}{\sum_j w_j M_j} \quad (60)$$

where:

- $E_i$  is the energy of the  $i$ -th species.
- $M_i$  is the atomic mass.
- $w_j$  is the statistical weight according to the stoichiometry of the molecule.

The constituents and the stoichiometry of the molecule are defined in the PDB.

You can define new molecular species with PDB commands. For example, you can define carborane as follows:

```
pdbSetString ImplantData Carborane Atom0 Name Boron
pdbSetDouble ImplantData Carborane Atom0 StWeight 10
pdbSetString ImplantData Carborane Atom1 Name Hydrogen
pdbSetDouble ImplantData Carborane Atom1 StWeight 14
```

Then, to initialize the species, use:

```
implant species= Carborane dataset= Boron
```

After the above two steps are performed, you can use carborane like any other predefined implantation species. For example, use the following command to perform analytic implantation for carborane:

```
implant Carborane energy= 10 dose= 1e14
```

**NOTE** The dose specified for analytic molecular implantation is the dose for the molecular species. In the above example, the implanted dose for carborane is  $1 \times 10^{14} \text{ cm}^{-2}$ . Therefore, the boron dose is  $1 \times 10^{15} \text{ cm}^{-2}$ , and the hydrogen dose is  $1.4 \times 10^{15} \text{ cm}^{-2}$ .

Sentaurus Process predefines the following molecular species: AsH<sub>2</sub> (AsH2), BCl<sub>2</sub> (BCl2), BF<sub>2</sub> (BF2), B<sub>18</sub>H<sub>22</sub> (B18H22), C<sub>2</sub>B<sub>10</sub>H<sub>12</sub> (C2B10H12), C<sub>2</sub>B<sub>10</sub>H<sub>14</sub> (C2B10H14), and PH<sub>2</sub> (PH2).

Depending on whether the implantation tables are supplied for the molecular species, analytic molecular implantation can proceed in two different ways:

- With implantation tables
- Without implantation tables

## Molecular Implantation With Implantation Tables

If implantation tables are available for the molecular species, the implantation proceeds in the same way as the atomic species; in other words, the specified energy and dose are used to look up the moments in the implantation tables. No scaling is applied to the energy, the dose, or the resulting profiles.

The implantation tables can be specified for a molecular species using:

```
implant species=<c> <material> imp.table=<c> dam.table=<c>
```

The implantation data files must be located in the current working directory or the full path to the file must be specified in `imp.table`.

## Molecular Implantation Without Implantation Tables

If implantation tables are not available for the molecular species, Sentaurus Process performs an approximate calculation of the dopant distribution using the implantation tables for the primary dopant species. The energy  $E_i$  for the  $i$ -th species (which is assumed to be the primary dopant species) is calculated using [Eq. 60, p. 102](#).

Assuming that there are  $N_i$  dopant atoms in a molecule, the molecular implantation is equivalent to a single atomic species implantation with the energy and dose equal to  $E_i$  and  $N_i \times \text{dose}$  (where `dose` is the molecular dose), respectively.  $E_i$  and  $N_i \times \text{dose}$  are used to look

### 3: Ion Implantation

#### Analytic Implantation

up the implantation moments. Then, the dopant distribution is calculated in the same way as for atomic implantation.

## Boron Difluoride Implantation

$\text{BF}_2$  is a special molecular species in analytic implantation because both boron and fluorine distributions are calculated in Sentaurus Process. By default, the fluorine profile is simply a boron profile multiplied by two. However, you can use the following switch to enable the separate calculation of fluorine distribution using the fluorine implantation tables:

```
pdbSet ImplantData BF2 TS4FluorineMode 1
```

When `TS4FluorineMode` is true, the fluorine profile is computed using the fluorine implantation tables in the same way as for TSUPREM-4.

## Damage Calculation

If damage tables are not supplied for the molecular species, the damage also can be calculated using the internal damage tables for the primary dopant species. The Boolean parameter `FullDamage` can be used to control the amount of damage for the molecular species:

```
pdbSetBoolean ImplantData <molecule> FullDamage <1 | 0>
```

If `FullDamage` is true, the calculated damage is multiplied by a scaling factor:

$$S_i = \frac{\sum w_j M_j}{M_i} \quad (61)$$

This damage scaling factor approximately takes into account the damage produced by all atomic species (including the primary dopant species) and is consistent with the damage calculation used in TSUPREM-4 for  $\text{BF}_2$  implantation.

---

## 1D or 2D Analytic Implantation in 3D Mode

Because analytic implantation performs lateral integration differently for one, two, and three dimensions, it may result in slightly different profiles from vertical 1D cuts, even though the same implantation moments are used. In addition, for a 2D structure, the vertical 1D profiles also may be different depending on the beam direction on the simulation plane or not, in other words, depending on the rotation angles.

To obtain the same results in any dimension or with different rotation angles, Sentaurus Process provides an option to perform 1D or 2D analytic implantation in 3D mode, in which case, a 1D

or 2D structure is first extruded into a pseudo-3D structure. In other words, only the surfaces and interfaces (not the bulk) are extended in the y-direction, or z-direction, or both directions, with the boundary conditions being taken into account.

In the case of PAI, damage integration is performed in a real 1D or 2D structure. Then, the lateral integration proceeds in exactly the same way as in a 3D analytic implantation. This ensures consistent results for 1D, 2D, and 3D implantations.

To switch on this option, use either `extrude` in the `implant` command or the global switch:

```
pdbSet ImplantData Extrude 1
```

## Implantation on (110)/(111) Wafers Using (100) Implantation Tables

Sentaurus Process typically includes a large set of implantation tables for Si(100) wafers, but it does not include any implantation tables for Si(110) or Si(111) wafers. However, you sometimes need to perform process simulations on (110) or (111) wafers.

Since the Si(100) implantation moments cannot be used directly for Si(110) or Si(111) wafers, certain transformations of implantation moments are required to use these tables for Si(110) or Si(111) wafers.

Since SIMS depth profiles are measured along the wafer normal direction, the extracted implantation moments also are obtained with respect to the wafer normal direction. On the other hand, analytic implantation is usually calculated using the beam direction as its primary direction. If the beam direction is coincidental with the normal direction, the implantation moments can be used directly without modification. However, for tilt implantations, the beam direction does not coincide with the wafer normal direction. In this case, implantation moments to be applied to the primary beam direction must be scaled, or transformed, to reproduce the 1D profiles in the wafer normal direction (see [Primary Direction and Scaling on page 87](#)).

Essentially, the projected range  $R_P$  is scaled as follows:

$$R'_P = R_P \cdot s_r \quad (62)$$

where  $s_r$  is the scaling factor shown in [Table 9 on page 89](#), and the primary standard deviation  $\sigma_p$  is scaled as follows:

$$\sigma'_p = \sqrt{s_r^2 \cdot \sigma_p^2 + (1 - s_r^2) \cdot \sigma_l^2} \quad (63)$$

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#### Analytic Implantation

To use Si(110) implantation tables for Si(110) or Si(111) implantations, you must calculate the corresponding angles on the (100) wafers from the specified implantation angles on the (110) or (111) wafers. For typical implantations (for example,  $\text{tilt}=7^\circ$ ), these angles are very large.

When you know the corresponding angle on the (100) wafer, you can use [Eq. 62](#) and [Eq. 63](#) to transform  $R_p$  and  $\sigma_p$ . [Eq. 62](#) works by simple geometry consideration. [Eq. 63](#) works reasonably well for small tilt implantations and, in theory, is accurate for isotropic amorphous material. However, due to ion channeling, [Eq. 63](#) may not be good under all situations.

Therefore, the following options for  $\sigma_p$  scaling are provided:

- Case 0 (constant):  $\sigma'_p = \sigma_p$
- Case 1 (linear):  $\sigma'_p = \sigma_p \cdot s_r$
- Case 2 (standard):  $\sigma'_p = \sqrt{s_r^2 \cdot \sigma_p^2 + (1 - s_r^2) \cdot \sigma_l^2}$

The default  $\sigma_p$  scaling is the same as the  $R_p$  scaling (linear scaling). These cases can be selected using the command:

```
pdbSet ImplantData StdevScalingMode {0 | 1 | 2}
```

---

## Multithreaded Parallelization of 3D Analytic Implantation

Parallel processing has become ubiquitous with the advent of multicore processors. The performance of 3D analytic implantation can be improved dramatically by exploiting the parallel processing power of multicore processors. In multithreaded mode, each thread works on separate nodes, sharing the workload, thereby reducing the computation time.

To engage the multithreaded parallelization of 3D analytic implantation, use the `math` command (see [math on page 1073](#)):

```
math numThreads=<i> | numThreadsImp3d=<i>
```

where `numThreads` is a general argument for 3D analytic implantation and MC implantation. However, `numThreadsImp3d` has a higher priority over `numThreads` for 3D analytic implantations and can be used to create the number of threads specifically for 3D analytic implantation, which is different from that for other multithreaded operations. The value of `numThreads` or `numThreadsImp3d` must equal the number of cores in multicore processors.

You also can modify the stack size for each thread using the command:

```
math threadStackSize=<i>
```

The default stack size ( $2^{18} = 262144$  bytes) is usually sufficient for 3D analytic implantation.

---

## Monte Carlo Implantation

This section describes Monte Carlo (MC) ion implantation.

---

### Running Sentaurus MC

Sentaurus Process can perform an atomistic simulation of ion implantation using the Monte Carlo simulator Sentaurus MC. MC implantation simulates ion implantation into single-crystalline materials or amorphous materials of arbitrary composition. In Sentaurus Process, to select MC implantation on the command line, use:

```
implant <species> sentaurus.mc
```

Alternatively, to select MC implantation as the default implantation model, use a global switch:

```
pdbSet ImplantData MonteCarlo 1
```

When MonteCarlo is set to 1, Sentaurus Process performs all the implantations using Sentaurus MC.

Fundamental parameters, such as the implantation energy and the dose, and the orientation of the ion beam with respect to the substrate must be specified using `energy`, `dose`, `tilt`, and `rotation` in the same way as for analytic implantation.

To run MC implantation in full-cascade mode or using the improved BCA (iBCA) damage model, use the `cascades` or `iBCA` switch:

```
implant <species> sentaurus.mc [cascades] [iBCA]
```

or use a global switch:

```
pdbSet MCImplant cascades 1  
pdbSet MCImplant iBCA 1
```

In the KMC mode, to specify the dose rate of the implantation, use `dose.rate`:

```
implant <species> sentaurus.mc [cascades] [iBCA] dose.rate=<n>
```

If `dose.rate` is specified, it is assumed to be a uniform dose rate in units of  $\text{cm}^{-2}/\text{s}$ . If it is not specified, a Tcl procedure will be called:

```
fproc DoseRate {dose} {...}
```

which returns an implantation time as a function of implantation `dose`. By default, it is a uniform dose rate; that is, `DoseRate` is a linear function of `dose`. However, you can specify

### 3: Ion Implantation

#### Monte Carlo Implantation

any monotonic function to take into account the particular implantation equipment setup or scanning patterns.

During the implantation, pseudoparticles representing a part of the whole dose start from the start surface, which is constructed above the target, parallel to the wafer surface. For 2D and 3D target geometries, the start surface is subdivided into segments of equal size for which the required implantation dose is accumulated. The size of these segments is controlled by setting:

```
 pdbSet MCImplant Intervals dy <n>
 pdbSet MCImplant Intervals dz <n>
```

**NOTE** Generally, dy and dz are not recommended to set to small values (default is  $0.05\text{ }\mu\text{m}$ ), since these parameters need, at least, a few times lateral straggling to make the errors caused by trajectory replication negligible.

For 1D structures, no subdivision is performed. The number of pseudoparticles that will start per segment can be set in the parameter database or on the command line:

```
 pdbSet MCImplant Particles <n>
```

or:

```
 implant <species> sentaurus.mc particles=<n>
```

The default value is 1000. Increasing this number leads to better accuracy and an increase in simulation time. Together with the sizes of the segments, particles determines the statistical weight of each pseudoparticle.

For KMC simulations, the number of particles ( $n$ ) per segment is computed automatically using the formula  $n = \text{dose} \cdot \text{dy} \cdot \text{dz} \cdot \cos(\text{tilt})$ .

**NOTE** For KMC simulations, it is recommended to set dy and dz to the domain dimensions to achieve the best accuracy. In the case of a small value for dy or dz, or a low dose, or a high tilt angle, the computed number of particles can be less than 1, in which case, a warning message is issued and the number is rounded up to one particle.

Launching particles are assumed to travel along the direction as specified by the tilt and rotation angles. However, there is usually a small angular divergence of the ion beam so that the particles form a right circular cone in which particles are assumed to be uniformly distributed. To specify the beam divergence angle (the angle between the cone axis and the cone surface), use:

```
 pdbSet MCImplant BeamDivergence <n>
```

Parameters controlling the electronic and nuclear stopping as well as the damage accumulation are available in the parameter database. You can set these parameters in the parameter database (see [Parameter Database on page 21](#)).

If the information level is set to 1 or more, a progress report similar to the following will be shown during the progress of the implantation:

implanted particles	orig traject	equiv classes	active segm	repl OK	traject fail	CPU step	time total
1300 ( 5%)	84	4	26	1216	6	0.22	0.22
2600 ( 10%)	170	4	26	2430	9	0.21	0.43
3900 ( 15%)	262	4	26	3638	16	0.21	0.64
5200 ( 20%)	349	4	26	4851	24	0.30	0.94
6500 ( 25%)	437	4	26	6063	29	0.47	1.41
7800 ( 30%)	523	4	26	7277	33	0.28	1.69
.....	.....	.....	.....	.....	.....	.....	.....
22100 ( 85%)	1894	4	5	20206	131	3.15	7.27
23400 ( 90%)	2875	4	5	20525	272	5.20	12.47
24700 ( 95%)	3837	4	5	20863	394	4.75	17.22
24960 ( 96%)	4029	4	5	20931	419	0.99	18.21
25220 ( 97%)	4231	4	5	20989	453	1.13	19.34
25480 ( 98%)	4422	4	5	21058	472	0.90	20.24
25740 ( 99%)	4628	4	1	21112	483	0.93	21.17
26000 (100%)	4888	4	0	21112	483	0.45	21.62
.....	.....	.....	.....	.....	.....	.....	.....
<b>Pseudo particles:</b>							
implanted : 26000							
lost : 0 (0%)							
Trajectories : 4888							
Equivalence classes: 4							

where:

- **implanted particles:** The total number of pseudoparticles implanted, which is, at the end of the simulation, equal to the product of the specified number of particles and the total number of segments of the implantation surface. This number includes both the calculated number of particles and the successfully replicated number of particles. The percentage of already finished particles is also indicated in parentheses.

**NOTE** In a multithreaded implantation, the thread ID also is shown before the percentage. For example, 6500 (2: 25%) means that thread #2 has implanted 6500 particles and is 25% finished.

- **orig traject:** The original number of trajectories that are based on the physical calculations.
- **equiv classes:** The number of equivalence classes in the current structure as detected by probing ions (see [Trajectory Replication on page 147](#)).

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- **active segm:** The number of currently active segments of the implantation surface. At the beginning of the implantation, this number equals the total number of start segments. This number should decrease as the implantation progresses. At the end of the implantation, the number becomes zero because all segments have the required implantation dose and are deactivated.
- **repl traject (OK and fail):** The number of replicated trajectories. The number of successfully replicated trajectories is shown in the `OK` column; whereas, the number of unsuccessful trajectories is shown in the `fail` column.
- **CPU time (step and total):** This CPU time includes the time spent for the current step and the total CPU time for the current implantation.

For 2D structures, the progress of an ion implantation step can be graphically viewed using `ion.movie`, for example:

```
implant <species> [sentaurus.mc] ion.movie
```

---

## Structure of Target Materials

MC implantation simulates the motion of energetic particles in single-crystalline materials and amorphous materials.

### Composition

For each material, the composition is set in the parameter database. The composition can be found in the `<material> -> Composition` entry.

For each `<n>`-component of the material, the entry `Component<n>` gives the name and the stoichiometric weight, which is generally the subscript of the component in a chemical (molecular) formula. For example, for gallium arsenide (GaAs):

```
GaAs -> Composition -> Component0 -> Name = Gallium  
GaAs -> Composition -> Component0 -> StWeight = 1  
  
GaAs -> Composition -> Component1 -> Name = Arsenic  
GaAs -> Composition -> Component1 -> StWeight = 1
```

or for silicon nitride (Si3N4):

```
Nitride -> Composition -> Component0 -> Name = Silicon  
Nitride -> Composition -> Component0 -> StWeight = 3  
  
Nitride -> Composition -> Component1 -> Name = Nitrogen  
Nitride -> Composition -> Component1 -> StWeight = 4
```

The composition for both single-crystalline and amorphous materials is set in this way.

## Single-Crystalline Materials

### Lattice Structure

In the case of a single-crystalline material, the positions of target atoms are calculated based on the lattice system and the polytype. Sentaurus MC supports several lattice systems including cubic, orthorhombic, and hexagonal. To specify the lattice system, use:

```
mater name=<c> [cubic | hexagonal | orthorhombic]
```

### Polytypes

To completely specify a lattice structure, in addition to the lattice system, you must specify the polytype:

- For cubic or orthorhombic systems, the following polytypes can be specified: Sc (simple cubic), Bcc (body-center cubic), Fcc (face-center cubic), and Zincblende (zinc-blende).
- For hexagonal systems, the following polytypes can be specified: 2H, 3C, 4H, and 6H.

To specify a polytype, use either:

```
mater name=<c> [cubic | orthorhombic] (polytype= Sc | Bcc | Fcc | Zincblende)  
mater name=<c> hexagonal (polytype= 2H | 3C | 4H | 6H)
```

The default polytype for silicon carbide (SiC) is 4H. For details, see [Monte Carlo Implantation Into Silicon Carbide on page 134](#).

### Lattice Constants

For all lattice systems, Sentaurus MC supports different lattice constants for three different axes. Lattice constants for crystalline materials can be defined using the `mater` command:

```
mater name=<c> lattice.const=<n> lattice.const.b=<n> lattice.const.c=<n>
```

The unit of the lattice constants is micrometer in the `mater` command. If `lattice.const.b` or `lattice.const.c` is not defined, it is assumed to be the same as `lattice.const`. In addition, for a hexagonal system, `lattice.const.b` must be equal to `lattice.const`.

### Atomic Basis Vectors

The crystal structure consists of the lattice sites plus a group of atoms. An atom *basis* can be a single atom or a group of atoms attached to each lattice site.

In Sentaurus MC, the undisturbed positions of the lattice sites are constructed automatically using the information of the lattice system, the polytype, and the lattice constants. Then, an atom or a group of atoms is assigned to each lattice site.

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#### Monte Carlo Implantation

For simple crystals (such as a single-atom basis with simple cubic, face-centered cubic, or body-centered cubic lattice, or binary compounds with zinc-blende and hexagonal lattice), each lattice site is occupied by one atom only. In this case, the atomic basis need not be specified as it has the same positions as the lattice sites.

For more complex crystal structures, the positions of basis atoms should be specified with the PDB parameter `BasisVector`. The units of basis vectors are lattice constants in the three crystallographic axes. Note that for each atom type, only one basis vector needs to be specified. Sentaurus MC automatically shifts and adds the other positions according to the symmetry of the structure. For example, for zinc-blende silicon, only two basis vectors, (0, 0, 0) and (0.25, 0.25, 0.25), need to be specified as follows:

```
Silicon -> Composition -> Component0 -> Name = Silicon
Silicon -> Composition -> Component0 -> StWeight = 1
Silicon -> Composition -> Component0 -> BasisVector = {0 0 0 0.25 0.25 0.25}
Silicon -> Composition -> Component0 -> BasisVector = {0 0 0 0.25 0.25 0.25}
```

The corresponding PDB commands are:

```
pdbSet Silicon Composition Component0 Name Silicon
pdbSet Silicon Composition Component0 StWeight 1
pdbSetDoubleArray Silicon Composition Component0 BasisVector
{0 0.0 0.0 0.0 1 0.25 0.25} ; # 0 and 1 are array indices
```

For another example, NaCl has a face-centered cubic (Fcc) lattice. Again, only two atomic basis vectors need to be specified, and these positions are shifted and added to their symmetric positions according to Fcc symmetry automatically. The positions of Na and Cl can be specified as follows:

```
NaCl -> Composition -> Component0 -> Name = Sodium
NaCl -> Composition -> Component0 -> StWeight = 1
NaCl -> Composition -> Component0 -> BasisVector = {0 0 0}

NaCl -> Composition -> Component1 -> Name = Chloride
NaCl -> Composition -> Component1 -> StWeight = 1
NaCl -> Composition -> Component1 -> BasisVector = {0.5 0.0 0.0}
```

The corresponding PDB commands are:

```
pdbSetString NaCl Composition Component0 Name Sodium
pdbSetDouble NaCl Composition Component0 StWeight 1
pdbSetDoubleArray NaCl Composition Component0 BasisVector {0 0.0 0.0 0.0}

pdbSetString NaCl Composition Component1 Name Chlorine
pdbSetDouble NaCl Composition Component1 StWeight 1
pdbSetDoubleArray NaCl Composition Component1 BasisVector {0 0.5 0.0 0.0}
```

## Thermal Vibrations

The thermal vibrations of the target atoms are important for the treatment of the motion of a projectile in single-crystalline material. In MC implantation, only instantaneous thermal displacements of target atoms from their ideal lattice sites are considered.

The displacements are assumed to obey a 3D Gaussian distribution with a root-mean-square obtained by the Debye model. The Debye temperature is set in the parameter database and can be changed with:

```
pdbSet <material> DebyeTemperature <n>
```

The default Debye temperature is 519 K for silicon.

The substrate temperature for the Debye model can be set by:

```
pdbSetDouble MCImplant Temperature <n>
```

The default substrate temperature is 300 K.

## Amorphous Materials

The structure of an amorphous material is described in a simplified manner by assuming an average interatomic distance in the target material.

You can use the MassDensity dataset as the mass density of an amorphous material:

```
pdbSetBoolean <material> VariableMassDensity 1
```

Using molar fractions is disabled in amorphous materials (see [Molar Fractions on page 114](#)).

## Polycrystalline Materials

A polycrystalline material is characterized by its crystal orientation and grain size. Crystal orientation (one of <100>, <110>, and <111>) can be specified using a material-specific command:

```
mater name= PolySilicon vertical.orient= {<n> <n> <n>}
```

There are two different ways to change the crystallinity (Amorphous, Crystalline, and Polycrystalline) of a material. If the parameter Crystallinity is available (which is true for polysilicon) in the PDB, use this switch to set the crystallinity, for example:

```
pdbSet PolySilicon Crystallinity Polycrystalline
```

### 3: Ion Implantation

#### Monte Carlo Implantation

This command makes MC implantation models consider both crystal orientation and grain size for polysilicon.

If Crystallinity does not exist for a material, use the Amorphous and Granular parameters:

```
pdbSet <material> Amorphous 0  
pdbSet PolySilicon Granular 1
```

The first command switches off the amorphous treatment, and the second command makes MC implantation models consider the grain size.

See [Monte Carlo Implantation Into Polysilicon on page 131](#).

## Molar Fractions

In Sentaurus Process, a mole fraction-dependent compound material is defined using a concentration field in a base material. For example,  $\text{Si}_{1-x}\text{Ge}_x$  is defined by either adding a germanium field in the base material silicon, or adding a silicon field in the base material germanium. As another example,  $\text{In}_{1-x}\text{Ga}_x\text{As}$  is defined by either adding a gallium field in the base material InAs, or adding an indium field in the base material GaAs.

See [Monte Carlo Implantation Into Alloy Materials on page 132](#).

---

## Physical Models of Sentaurus MC

The Sentaurus MC implantation engine is designed to be generally accurate and predictive with minimum user calibrations for most implantation conditions. It has been calibrated from sub-keV to above 10 MeV, and for different implantation conditions including random implantation direction,  $\langle 100 \rangle$ ,  $\langle 111 \rangle$ , and  $\langle 110 \rangle$  channeling directions, with the same set of parameters for boron, phosphorus, and arsenic implantations [3]. It also is accurate for other implantation species such as  $\text{BF}_2$ , C, N, F, Al, Ge, In, and Sb [3][14].

For a detailed discussion of the physical models of Sentaurus MC and an extensive comparison with experimental SIMS profiles from sub-keV to above 10 MeV and with other MC simulators, refer to the literature [3][14]. This section briefly outlines the pertinent theory and models.

The calculation used in Sentaurus MC assumes that ions lose energy through two processes:

- Nuclear scattering, where the nucleus of the ion elastically scatters off the nucleus of an atom in the target. This interaction is based on the binary collision theory (see [Binary Collision Theory on page 115](#)).

- Interaction of the ion with the electrons of the target atoms. This mechanism is inelastic and does not alter the direction of the motion of the ion.

Therefore, the total change in energy of the ion after the  $i$ -th collision is the sum of the nuclear energy loss  $\Delta E_n$  and the electronic energy loss  $\Delta E_e$ :

$$E_i = E_{i-1} - \Delta E_n - \Delta E_e \quad (64)$$

## Binary Collision Theory

Sentaurus MC implantation models the energy loss of nuclear collision according to the classical binary scattering theory. The basic assumption of the mechanism for the energy loss of nuclear collision is that the ion interacts with only one target atom at a time. This assumption enables the use of the binary scattering theory from classical mechanics [15].

BCA is valid in a wide range of projectile energies, from approximately 100 eV to many MeV. It can, therefore, be used over the whole range of energies of interest for ion implantation. For energies below approximately 100 eV, collective interactions may play an increasingly important role and BCA may become invalid. Nevertheless, the applications of Sentaurus MC simulation to ultralow-energy implantations lead to results that are still sufficiently good compared with experimental data.

Consider a particle of mass  $M_1$  and kinetic energy  $E_0$  approaching a stationary particle with mass  $M_2$ . The impact parameter  $b$  is the distance of closest approach if the particle is not deflected and gives a convenient measure of how close the collision is. After collision, the first particle deviates from its original course by an angle  $\theta$ .

## Energy Loss

It can be shown that the first particle loses kinetic energy:

$$\frac{\Delta E_n}{E_0} = \frac{4M_1 M_2}{(M_1 + M_2)^2} \cos^2(bI) \quad (65)$$

where:

- $\Delta E_n$  is the energy lost by particle 1.
- $E_0$  is its energy before collision.
- $I$  is the integral:

$$I = \int_0^{s_{\max}} \frac{ds}{\sqrt{1 - \frac{V(s)}{E_r} - b^2 s^2}} \quad (66)$$

### 3: Ion Implantation

#### Monte Carlo Implantation

where  $s = r^{-1}$  is the inverse separation between the two particles.  $V(s)$  is the potential between the two particles (assumed to be repulsive), and:

$$E_r = \frac{E_0}{1 + M_1/M_2} \quad (67)$$

is the reduced energy in the center of the mass coordinates.

The upper limit of the integral,  $s_{\max}$ , is the inverse distance of closest approach of the two particles and is given by the solution to the equation:

$$1 - \frac{V(s_{\max})}{E_r} - b^2 s_{\max}^2 = 0 \quad (68)$$

### Scattering Angle

The angle  $\theta$  by which particle 1 is deflected is given by:

$$\cos \theta = \frac{1 - 0.5 \left[ 1 + \frac{M_2}{M_1} \right] \Delta E_n / E_0}{\sqrt{1 - \Delta E_n / E_0}} \quad (69)$$

**NOTE** For  $\Delta E_n / E_0 \ll 1$ ,  $\theta$  approaches zero.

### Dimensionless Form

[Eq. 65](#) to [Eq. 69](#) are the basic equations for classical two-body scattering. The scattering integral, [Eq. 66](#), can be cast into a dimensionless form by assuming the potential has the form:

$$V(s) = Z_1 Z_2 k_1 s g(a_u s) \quad (70)$$

where:

- $Z_1$  is the charge on particle 1.
- $Z_2$  is the charge on particle 2.
- $k_1$  is the constant:  $k_1 = \frac{q^2}{4\pi\epsilon_0} = 14.39495 \times 10^{-7} \text{ keV}\mu\text{m}$ .
- $g(a_u s)$  is an arbitrary function of  $a_u s$ , to be defined later, and  $a_u$  is a unit of length. Sentaurus MC uses the so-called universal screening length [\[16\]](#):

$$a_u = 0.8854 \times 10^{-4} \frac{0.529}{(Z_1^{0.23} + Z_2^{0.23})} \mu\text{m} \quad (71)$$

and a dimensionless impact parameter:

$$b_n = \frac{b}{a_u} \quad (72)$$

and a dimensionless energy:

$$\epsilon = \frac{a_u E_r}{Z_1 Z_2 k_1} \quad (73)$$

Using Eq. 70, Eq. 72, and Eq. 73 in the scattering integral Eq. 66 and making the substitution  $s' = a_u s$  gives:

$$I = \frac{1}{a_u} \int_0^{s'_\text{max}} \frac{ds'}{\sqrt{1 - s' g(s')/\epsilon - b_n^2 s'^2}} \quad (74)$$

From Eq. 65, the quantity of interest is  $\cos^2(bI)$ , which becomes:

$$\cos^2(bI) = \cos^2 \left[ b_n \int_0^{s'_\text{max}} \frac{ds'}{\sqrt{1 - s' g(s')/\epsilon - b_n^2 s'^2}} \right] \quad (75)$$

Therefore, using Eq. 75,  $\cos^2(bI)$  can be evaluated in terms of the dimensionless variables  $b_n$  and  $\epsilon$ , without reference to the charge or mass of a particular particle.

## Coulomb Potential

As an example of the above procedure, consider the Coulomb potential between two particles:

$$V(r) = \frac{Z_1 Z_2 k_1}{r} \quad (76)$$

or:

$$V(s) = Z_1 Z_2 k_1 s \quad (77)$$

In this case,  $g(a_u s) = 1$ . Then, from Eq. 75:

$$\cos^2(bI) = \cos^2 \left[ b_n \int_0^{s'_\text{max}} \frac{ds'}{\sqrt{1 - s'/\epsilon - b_n^2 s'^2}} \right] \quad (78)$$

### 3: Ion Implantation

#### Monte Carlo Implantation

with:

$$s'_{\max} = \frac{\sqrt{1 + 4b_n^2\varepsilon^2} - 1}{2\varepsilon b_n^2} \quad (79)$$

from a solution of [Eq. 68](#).

Then, the integral can be evaluated exactly, giving:

$$\cos^2(bI) = \frac{1}{1 + 4b_n^2\varepsilon^2} \quad (80)$$

For a given impact parameter  $b$  and incident energy  $E_0$ , the dimensionless  $b_n$  and  $\varepsilon$  can be obtained from [Eq. 72](#) and [Eq. 74](#), giving  $\cos^2(bI)$  from [Eq. 80](#). Then, the energy loss due to the collision is given by [Eq. 65](#), and the angle at which particle 1 leaves the collision is given by [Eq. 75](#).

### Universal Potential

For the simple form of the Coulomb potential used in the previous example, the scattering integral can be solved analytically. For more realistic interatomic potentials, however, the scattering integral cannot be evaluated analytically.

For example, the universal potential [\[16\]](#) that is used in Sentaurus MC is:

$$V(r) = \frac{Z_1 Z_2 k_1}{r} [0.18175 e^{-3.1998 r/a_u} + 0.50986 e^{-0.94229 r/a_u} + 0.28022 e^{-0.4029 r/a_u} + 0.028171 e^{-0.20162 r/a_u}] \quad (81)$$

An analytic solution does not exist since the upper limit of the integral in [Eq. 66](#) is given by [Eq. 68](#), which becomes a transcendental equation with this potential.

In Sentaurus MC, the quantity  $\cos^2(bI)$ , in its dimensionless form ([Eq. 75](#)), is numerically integrated for a wide range of its parameters  $b_n$  and  $\varepsilon$ . These results are stored in tables. Then, at each collision,  $\cos^2(bI)$  is obtained from these tables. This scheme eliminates the need to find  $s_{\max}$  for each collision, minimizing the amount of arithmetic operations performed during the calculation of the trajectory of an ion, while retaining accuracy.

Tables for the universal potential over a wide range of energies and impact parameters are provided for immediate use in Sentaurus MC. These tables span the normalized energy range of  $10^{-5} \leq \varepsilon \leq 100$  and the normalized impact parameter range  $0 \leq b_n \leq 30$ . For  $\varepsilon > 100$ , the Coulombic form ([Eq. 81](#)) is used.

Values of  $\varepsilon < 10^{-5}$  are not encountered for ion–atom combinations of interest at energies above the energy at which the ion is assumed to have stopped (5 eV). For values of  $b_n > 30$ , the ion is assumed to be undeflected.

## Implantation Into Amorphous Materials

This section describes how the binary collision theory is used to calculate ion trajectories in an amorphous solid. Assume an ion with kinetic energy  $E_0$  hits a target with an angle  $\theta_0$  with respect to the target normal. The surface of the target is assumed to be at  $y = 0$ , with  $y$  increasing vertically into the target.

To set the incident energy  $E_0$  in the `implant` command, use the `Energy` argument. To specify the incident angle  $\theta_0$  in the `implant` command, use the `tilt` argument.

Given the atomic density  $N_{\text{dens}}$  for the target material, the mean atomic separation between atoms in the target is  $1/(N_{\text{dens}})^{1/3}$ . Between scattering events, the ion is assumed to travel a distance:

$$L = \frac{1}{(N_{\text{dens}})^{1/3}} \quad (82)$$

As the ion enters the target material, it approaches the first target atom with impact parameter  $b$ , defined in [Binary Collision Theory on page 115](#). The probability of finding a target atom between  $b$  and  $b + \delta b$  is given by:

$$w(b)\delta b = 2\pi N_{\text{dens}}^{2/3} b \delta b \quad (83)$$

for  $b < 1/\sqrt{\pi N_{\text{dens}}^{2/3}}$ .

If  $R_{\text{rand}}$  is a uniformly distributed random number between 0 and 1, the probability distribution gives:

$$b = \sqrt{\frac{R_{\text{rand}}}{\pi N_{\text{dens}}^{2/3}}} \quad (84)$$

Given the above definitions, the algorithm for calculating the energy loss through nuclear collisions experienced by the ion proceeds as follows:

- A random number between 0 and 1 is chosen.
- The normalized impact parameter for this collision is calculated from [Eq. 72](#) and [Eq. 84](#):

$$b = \frac{1}{a_u} \sqrt{\frac{R_{\text{rand}}}{\pi N_{\text{dens}}^{2/3}}} \quad (85)$$

### 3: Ion Implantation

#### Monte Carlo Implantation

- The ion energy  $E_0$  is normalized to:

$$\varepsilon = \frac{a_u E_0}{(1 + M_1/M_2) Z_1 Z_2 k_1} \quad (86)$$

from [Eq. 68](#) and [Eq. 73](#).

- Now, the value of  $\cos^2(bI)$  can be obtained from the implantation tables, and [Eq. 65](#) gives the energy loss due to nuclear scattering:

$$\Delta E_0 = \text{nucl.cor} \cdot E_0 \frac{4M_1 M_2}{(M_1 + M_2)^2} \cos^2(bI) \quad (87)$$

where `nucl.cor` is an empirical nuclear-scattering correction factor with a default value of 1.0, which can be changed in the parameter database using:

```
pdbSetDouble <material> <dopant> nucl.cor <n>
```

This procedure is repeated for each collision event.

## Implantation Into Crystalline Materials

The binary collision calculation for crystalline materials proceeds in the same way as for amorphous materials, except that the selection of the collision partners of the projectile with target atoms is conducted in a more sophisticated manner.

Instead of using the density of the target material and a random number, Sentaurus MC determines the collision partners based on the position of the projectile relative to the sites on an idealized lattice. The algorithm for selecting the collision partners is based on MARLOWE [17]. Sentaurus MC implantation uses a sophisticated *multibody* collision algorithm to simulate the collisions of well-channeled particles, as shown in [Figure 18](#).

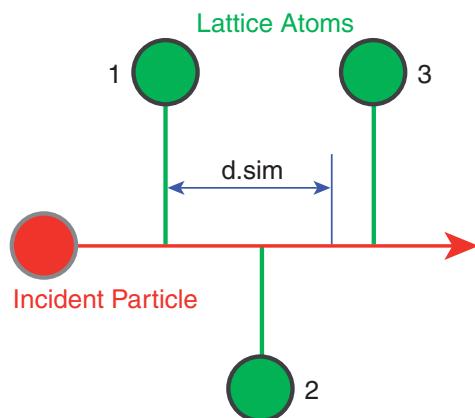


Figure 18 Illustration of simultaneous collision, and definition of `d.sim` argument

To find the collision partners, Sentaurus MC first collects all the lattice atoms that are within half the lattice constant of the incident particle and also in the forward direction of the incident particle. Then, these lattice atoms are projected to the moving direction of the incident particle. The closest atom (call it atom 1, for example) is then selected and, if the distance of one or more projected lattice atoms is less than `d.sim` (simultaneous collision distance in units of the lattice constant) from the projected position of atom 1, these atoms are also considered to be collision partners, and the multibody collision algorithm is invoked. For example, in [Figure 18 on page 120](#), 1 and 2 are considered to be *simultaneous* collisions, but 3 is not.

The default value of `d.sim` is 0.5 lattice constant for all crystalline materials except for SiC, which has a default value of 0.25 lattice constant. To change the value of `d.sim` for a material, use:

```
pdbSetDouble <material> d.sim <n>
```

The scattering events are computed for each target individually, and the final moment and energy of the incident particle are computed by applying momentum and energy conservation principles.

The simultaneous collisions are handled in the same way as for MARLOWE, except for the location of the turning point. In MARLOWE, the turning point is assumed to be the average of those of the simultaneous collision partners. In Sentaurus MC, the turning point is placed at a point determined by the collision with the minimum impact parameter.

Simulations have indicated that such a scheme obtains better results for ultralow energy implantations, while it has little impact on implantation energies above 5 keV. This allows Sentaurus MC to treat the entire implantation energy range, including ultralow energy and very high energy, with the same model, in exactly the same way.

Ion channeling, which is the preferential penetration of implanted ions along crystal axes or planes, occurs naturally due to the inclusion of the crystal structure of the lattice. Both axial and planar channeling show enhanced penetrations. The effect of the `tilt` and `rotation` arguments is much more pronounced for implantations into crystalline silicon than into amorphous silicon.

## Electronic Stopping Model

A moving ion loses energy by inelastic electronic processes, which include both nonlocal and local stopping power. Sentaurus MC uses the same electronic stopping model for both amorphous and crystalline materials.

### 3: Ion Implantation

#### Monte Carlo Implantation

For each collision, the energy loss due to electronic stopping is:

$$\begin{aligned}\Delta E_e &= x^{\text{nl}} \cdot \Delta E_e^{\text{nl}} + x^{\text{loc}} \cdot \Delta E^{\text{loc}} \\ x^{\text{nl}} + x^{\text{loc}} &= 1 \\ x^{\text{nl}} &= \min(\text{nloc.pre} \cdot \varepsilon^{\text{nloc.exp}}, 1)\end{aligned}\tag{88}$$

where  $\varepsilon$  is the scaled dimensionless energy.

Both `nloc.pre` and `nloc.exp` are specified in the material parameter database and can be changed using:

```
pdbSet <material> <dopant> nloc.pre <n>
pdbSet <material> <dopant> nloc.exp <n>
```

### Nonlocal Electronic Stopping

Nonlocal electronic stopping acts as the dragging (frictive) force on moving ions, which is proportional to the ion velocity and is independent of the impact parameter:

$$\begin{aligned}\Delta E_e^{\text{nl}} &= L \cdot N_{\text{dens}} \cdot S_e \\ S_e &= \text{LSS.pre} \cdot S_{es} \cdot \sqrt{E_m} \cdot f_{es}^{-1}\end{aligned}\tag{89}$$

where  $L$  is the free flight path between collisions, and  $E_m$  is the ion energy at the stopping power maximum.

You can specify `LSS.pre` in the material parameter database. To change it, use:

```
pdbSet <material> <dopant> LSS.pre <n>
```

The quantities  $S_{es}$  and  $f_{es}$  are given by [3][18]:

$$\begin{aligned}S_{es} &= \frac{1.212 Z_1^{7/6} Z_2}{[Z_1^{2/3} + Z_2^{2/3}]^{3/2} M_1^{1/2}} \\ f_{es} &= \left[ \left( \frac{E_0/E_m}{\ln(E_0/E_m + E_m/E_0 + e - 2)} \right)^{\delta/2} + \left( \frac{E_m}{E_0} \right)^{\delta/2} \right]^{1/\delta}\end{aligned}\tag{90}$$

where:

- $Z_1$  is the ion atomic number.
- $Z_2$  is the composite target atomic number.
- $e$  is the base of the natural logarithm.
- $\delta = 1.425$  is a fitting parameter.

## Local Electronic Stopping

Local electronic loss is the result of the electron exchange between the moving ion and the target atom, which is based on the Oen–Robinson model [19] and is dependent on the impact parameter:

$$\begin{aligned}\Delta E_e^{\text{loc}} &= \frac{S_e}{2\pi a^2} \cdot \exp\left(-\frac{b}{a}\right) \\ a &= f \cdot \frac{a_u}{0.3} \\ f &= \text{scr.par} \cdot \frac{1.45}{Z_1^{2/5}}\end{aligned}\quad (91)$$

where `scr.par` is an adjustable screening length parameter that you can change using:

```
pbSet <material> <dopant> scr.par <n>
```

## Damage Accumulation and Dynamic Annealing

As ions travel through a crystalline target, they collide with the target atoms and displace many of them from their lattice sites. In the binary collision approximation (BCA) code, it is assumed that, if the transferred energy exceeds a certain threshold, the target atom is displaced and, at this lattice site, a vacancy is generated.

When the displaced atom comes to rest, it is identified as an interstitial. This defect production rate can be evaluated either by the modified Kinchin–Pease formula [20] or by simulating the full cascade. Sentaurus MC provides both types of damage calculation.

### Damage Accumulation Models

The default damage model calculates the deposit energy  $E_D(x)$  for each collision, which is then converted to the number of point defects (Frenkel pairs) using the modified Kinchin–Pease formula [20]:

$$n(x) = \kappa \left( \frac{E_D}{2 \cdot \text{disp.thr}} \right) \quad (92)$$

where  $\kappa = 0.8$  and `disp.thr = 15 eV` for silicon by default.

If `cascades` is specified in the `implant` command, Sentaurus MC traces all of the generated secondary recoils. After each collision, a calculation is performed to determine the trajectories of the silicon lattice atoms that are knocked from their sites in the lattice by collisions with implanted ions. A silicon atom is assumed to be knocked from its site when it absorbs an energy greater than a damage threshold `casc.dis` from a collision.

### 3: Ion Implantation

#### Monte Carlo Implantation

The silicon atoms freed from the lattice can, in turn, knock other atoms from their sites so that cascades of damage result. Sentaurus MC calculates the trajectories of these knock-ions with the same detail as the implanted ions. A vacancy is assumed to have formed whenever a lattice atom is knocked from its site. An interstitial is assumed to have formed whenever a silicon lattice atom that has been knocked from its site comes to rest. This damage model can be used to calculate the different profiles of interstitials and vacancies, that is, I-V separations.

Both `disp.thr` and `casc.dis` are specified in the material PDB, and you can change them using:

```
 pdbSet <material> <dopant> disp.thr <n>
 pdbSet <material> <dopant> casc.dis <n>
```

Ideally, the displacement threshold should remain the same for all implanted species in a given material. However, for the purpose of calibration, for each dopant species, you can specify an individual displacement threshold. A question arises regarding the full cascade damage model (using silicon as an example): When a silicon atom is displaced by another silicon atom, which displacement threshold should be used (that of the dopant or that of silicon)?

The default behavior is to use the displacement threshold of the dopant, which has the following advantages:

- Different dopant species are decoupled from each other when performing calibration.
- The damage parameters can be transferred easily from the default (noncascade) damage model to the cascade damage model.

However, if the model is fully calibrated, using the displacement threshold of silicon for all implanted species would help find a better set of damage parameters. To decouple or couple different dopant species, use the following command:

```
 pdbSet MCImplant Cascades.Damage.Model {Decoupled | Coupled}
```

So far, for the purpose of calibration, for each dopant species, you can specify its own displacement threshold. However, this displacement threshold is the same for each component of the material. Ideally, the displacement threshold is associated with a specific material, and each component of the material could have its own displacement threshold, and these should remain the same for all implanted species.

To specify a different displacement threshold for each different component in compound materials, you must switch on the following PDB command:

```
 pdbSet MCImplant Individual.Displace.Threshold 1
```

In addition, you must specify the displacement for each component as follows:

```
 pdbSetDouble <material> Composition Component<n> disp.thr <n>
```

For example, for silicon carbide, you can specify the following:

```
pdbSetDouble SiC Composition Component0 disp.thr <n1>
pdbSetDouble SiC Composition Component1 disp.thr <n2>
```

where the displacement threshold for the silicon component takes the `<n1>` value, while that for the carbon component takes the `<n2>` value.

**NOTE** When `Individual.Displace.Threshold` is switched on, you must specify the displacement threshold for each component, which can have different values. However, these displacement threshold values will be the same for all implanted species.

## Dynamic Annealing

Not all of the defects as calculated above will survive. Some of the generated defects will recombine within the cascade as well as with the pre-existing defects. To achieve computational efficiency, Sentaurus MC uses a statistical approach to account for the I–V recombination in both intracascades and intercascades. The encounter probability of the projectile with interstitials also is accounted for statistically. The net increase of the defects in a local region with defect concentration  $C(x)$  is:

$$\Delta n(x) = \text{surv.rat} \cdot n(x) \cdot \left(1 - \frac{\text{sat.par} \cdot C(x)}{N_{\text{dens}}}\right) \quad (93)$$

In the cascade damage model, `surv.rat` and `sat.par` are replaced with `casc.sur` and `casc.sat`. To conserve particle numbers, interstitials and vacancies are recombined in pairs, and the model distinguishes between recoiled interstitials and recoiled lattice atoms. When an interstitial is recoiled, the local interstitial number decreases by one and no vacancy is produced. On the other hand, when a lattice atom is recoiled, a vacancy is created. However, defect recombination must be considered.

The intracascade recombination is accounted for by a factor `casc.sur`, while intercascade recombination is accounted for by a probability  $1 - (N_I/N_{\text{dens}})$ , which describes that the vacancy is not located within the capture radius of an interstitial.

When a recoil comes to rest, it is only allowed to recombine with vacancies from previous cascades, which is described by a factor  $1 - (N_V/N_{\text{dens}})$ , but not with those of the same cascade since this recombination has already been accounted for by vacancy intracascade recombination in the previous step.

Both `surv.rat` and `casc.sur` are specified in the material PDB, and you can change them using:

```
pdbSet <material> <dopant> surv.rat <n>
pdbSet <material> <dopant> casc.sur <n>
```

### 3: Ion Implantation

#### Monte Carlo Implantation

For light implantation species, damage could saturate at certain concentrations due to the balance between defect production and dynamic annealing. Damage saturation is controlled by the parameters `sat.par` and `casc.sat` for the default damage model and cascade damage model, respectively. The default value is 1 for all implantation species. Therefore, with the default parameter, the maximum damage is equal to the lattice density.

If, for example, `sat.par` is set to 4.35, damage saturates at 23% of the lattice density and cannot exceed the amorphization threshold ( $1.15\text{e}22 \text{ cm}^{-3}$  by default). Therefore, the crystal will never be amorphized in this case. To change these parameters, use:

```
pdbSetDouble <material> <dopant> sat.par <n>
pdbSetDouble <material> <dopant> casc.sat <n>
```

**NOTE** For heavy species, a single cascade may amorphize the crystal. Therefore, the intracascade parameter `sat.par` may not prevent the amorphization even if it is set to a very large value.

#### Damage De-Channeling

The accumulated damage has a significant effect on the destination of the subsequent ions, thereby altering the shape of the impurity profiles. This effect is known as *damage de-channeling*. Sentaurus MC handles this problem by switching from the crystalline model to the amorphous model based on the damage that has accumulated in the substrate. If the local defect concentration  $C(x)$  is greater than the amorphization threshold, this local region is assumed to be amorphized, and the amorphous collision model is used for this local region.

For the local regions with defect concentrations below the amorphization threshold, the probability of selecting the amorphous model is proportional to the local defect concentration  $C(x)$  and a random number call. The amorphous collision model is selected when:

$$R_{\text{rand}} < \text{amor.par} \cdot \frac{C(x)}{N_{\text{dens}}} \quad (94)$$

Increasing `amor.par` makes the profiles more like those implantations into amorphous materials. For the cascade damage model, `amor.par` is replaced with `casc.amo`. The parameters `amor.par` and `casc.amo` are specified in the material PDB, and you can change them using:

```
pdbSet <material> <dopant> amor.par <n>
pdbSet <material> <dopant> casc.amo <n>
```

**NOTE** For low-energy implantations, due to very shallow projected ranges, the mesh near the surface must be refined to account fully for the damage de-channeling effect.

**NOTE** Sentaurus MC does not explicitly simulate the amorphization process. However, for Sentaurus MC, by common practice, when a critical amount of damage accumulates in a certain region, a crystal/amorphous phase transition is assumed to occur in that region. For a silicon target, this critical amorphization threshold is approximately 25% of the lattice density. Therefore, if the defect concentration reaches more than  $1.15 \times 10^{22} \text{ cm}^{-3}$  for silicon, this region is considered to be amorphized. Using this criterion, Sentaurus MC predicts the onset of amorphization and the thicknesses of the amorphous layers for high-dose implantations.

## Improved Binary Collision Approximation Damage Model

During implantation, energetic ions penetrate the target and lose their energy through collisions with atoms and electrons. It is traditionally assumed that only energy deposited in the form of nuclear collisions contributes to damage generation; whereas, energy transfers to the electronic system are taken as inelastic losses. While energetic atoms are in the ballistic regime (that is, they have energies well above the displacement threshold `casc.dis`), they can be well simulated using binary collision approximation (BCA) algorithms. However, as their energy decreases to the thermal regime (around and below the displacement threshold), multiple interactions with target atoms become important. Molecular dynamics (MD) simulations demonstrate that energy transfers among atoms at this low-energy regime can generate amorphous pockets, thereby generating more damage than BCA models. The improved BCA (iBCA) damage model is an attempt to simulate MD simulation results within the framework of BCA.

The iBCA damage model implemented in Sentaurus MC is largely based on Santos *et al.* [21] (for the detailed physical basis of the model, refer to this article).

This section briefly describes the model, its usage, and the parameters that are accessible to users.

The procedure followed in the iBCA model is:

1. The collision phase of the cascade is simulated with the conventional BCA model.
2. The BCA simulation provides the position of Frenkel pairs generated during the cascade, the remaining energy of the recoils at the end of their trajectories, and the position and energy of all atoms that receive any amount of energy above the minimum energy (`MinHotEnergy`). These particles are *hot particles*.
3. At the end of the collision phase, there is a set of vacancies, interstitials, and hot particles.

### 3: Ion Implantation

#### Monte Carlo Implantation

Within the BCA, the energy conservation principle applied to elastic binary collisions implies that the energy of the incident particle must be equal to its energy after the collision plus the recoil energy plus the energy required to take the recoil away from its lattice site.

A moving atom stops when its energy is insufficient to generate more subcascades. However, the remaining energy of the generated interstitial at the end of its trajectory can still contribute to generate more damage if low-energy interactions were modeled. To consider this effect within the iBCA model, the residual energy of each generated interstitial is shared equally with its neighboring atoms. Ballistic collision only considers the impinging atom and the closest target atom (two-body interactions). However, as energy decreases, collisions with several target atoms occur more often, and groups of energetic atoms are created as the cascade develops (manybody interactions).

After this energy rearrangement, you evaluate which atoms are disordered taking into account their efficiencies:

$$\text{efficiency} = \frac{\rho - E_T}{D_C} \quad (95)$$

where  $\rho$  is the energy density, and  $E_T$  and  $D_C$  are the threshold energy density and the damage generation cost, respectively. If the calculated efficiency of a given atom is below zero, it is not disordered.

If *efficiency* is between 0 and 1, the atom is disordered with a random probability given by its efficiency. If *efficiency* is 1 or greater, the atom is disordered and a random neighbor is disordered with the probability given by the remaining efficiency (*efficiency* – 1) and so on.

To simulate the energy diffusion process: First, evaluate the efficiency of those atoms with the highest amount of energy in their environment. Second, repeat the process until no more energy remains to create more disordered atoms.

This scheme for damage generation can be regarded as a combination of the two traditional BCA approaches for damage description. As in the full-cascade BCA, ion and recoil trajectories are followed to generate damage at the atomic level and to provide the individual positions of Frenkel pairs, but you also must consider the energy deposited in atoms not displaced by ballistic collisions. This energy is used to generate thermally disordered atoms following a scheme similar to the modified Kinchin–Pease approach. Nevertheless, since the residual deposited energies that are being considered to determine efficiencies are always at the low-energy regime, the local character of damage generation is guaranteed. In addition, the damage efficiency expression accounts for phase transformation (melting) and heat dissipation through the dependency of the parameters  $E_T$  and  $D_C$  on the number of energetic neighbors. This feature captures the nonlinear effects on damage generation due to the proximity of several energetic atoms as it occurs in molecular implantation.

To activate the iBCA damage model, specify `iBCA` in the `implant` command or use the global switch:

```
pdbSet MCImplant iBCA 1
```

You can calibrate the iBCA damage model by changing the minimum energy for hot particles (`MinHotEnergy`) and the maximum distance for the local neighbors (`DistLocalNeighbors`):

```
pdbSet Silicon MinHotEnergy <n>
pdbSet Silicon DistLocalNeighbors <n>
```

By default, `MinHotEnergy` is 1 eV, and `DistLocalNeighbors` is 3.84e-4 μm.

In addition, you can calibrate the model by changing the formulas for the threshold energy density (`Et_iBCA`) and the damage generation cost (`Dc_iBCA`) by modifying Tcl procedures. As noted in [21], the default Tcl procedures for these quantities are defined as (where `ln` is the number of local neighbors):

```
fproc Et_iBCA { ln } {
    set et [expr 11.348 * pow($ln+1, -0.837) + 0.931]
    return $et;
}

fproc Dc_iBCA { ln } {
    set dc [expr 11.211*exp(-0.146*$ln + 0.00158*$ln*$ln)];
    return $dc;
}
```

**NOTE** To avoid nonphysical results, only fine-tuning of these formulas is recommended.

**NOTE** Because the iBCA damage model is substantially more CPU intensive than the cascade damage model, only low-energy implantation is practical for this damage model.

---

## Monte Carlo Molecular Implantations

The MC method allows for the implantation of molecular ions or atomic cluster species such as BF2. The assumption is that the molecule immediately breaks up into its constituents upon impact on a solid surface.

### 3: Ion Implantation

#### Monte Carlo Implantation

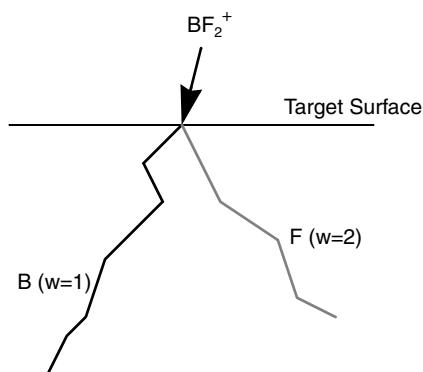


Figure 19 Schematic of molecular implantation of  $\text{BF}_2$ : one trajectory is calculated for each atomic species, and  $w$  is the weight assigned to the species

This is a valid approximation if the binding energy of the molecule is considerably smaller than the implantation energy (for example, for  $\text{BF}_2$ :  $E_B \sim 9$  eV).

The implantation energy is shared by several atoms according to:

$$E_i = \text{energy} \cdot \frac{M_i}{\sum_j w_j M_j} \quad (96)$$

where:

- $E_i$  is the energy of the  $i$ -th species.
- $M_i$  is the atomic mass.
- $w_j$  is the statistical weight according to the stoichiometry of the molecule.

The constituents move as separate particles. However, particles of different species are not completely independent because of the interaction through implantation damage.

Sentaurus Process supports several molecular species:  $\text{BF}_2$  (BF2),  $\text{BCl}_2$  (BCl2),  $\text{B}_{18}\text{H}_{22}$  (B18H22),  $\text{AsH}_2$  (AsH2), and  $\text{PH}_2$  (PH2).

For example, an implantation of  $\text{B}_{18}\text{H}_{22}$  can be performed with:

```
implant B18H22 energy= 100 sentaurus.mc
```

The atomic masses, the statistical weights, and the molecular composition are available in the parameter database. A full MC molecular implantation is performed if `full.molecular` is explicitly specified, for example:

```
implant <dopant> sentaurus.mc full.molecular
```

In this case, the trajectories of all atomic species are calculated. At the end of the simulation, datasets for each ballistic constituent of the original molecule are generated. This is the default. Only the trajectory of the significant species (B in the case of BF<sub>2</sub>) is calculated if !full.molecular is specified.

---

## Monte Carlo Implantation Into Polysilicon

Polysilicon has three states of crystallinity:

- Amorphous
- Crystalline
- Polycrystalline

By default, polysilicon is considered amorphous and can be treated as a single-crystalline or polycrystalline material using:

```
pdbSet PolySilicon Crystallinity Crystalline  
pdbSet PolySilicon Crystallinity Polycrystalline
```

Crystal orientation (one of <100>, <110>, and <111>) can be specified using the mater command, for example:

```
mater name=PolySilicon vertical.orient= {1 1 0}
```

This command sets the vertical orientation for all polysilicon regions to <110>.

If crystallinity is set to Polycrystalline, MC implantation checks for the existence of the GSize dataset or the GrainSize parameter. If neither is found, the grain model is disabled, and the material is assumed to be single crystalline. The default grain size is  $5 \times 10^{-5}$  [cm], and it can be changed with the command:

```
pdbSet PolySilicon GrainSize <n>
```

or by initializing the GSize dataset:

```
select z=<n> name= GSize
```

The unit for both GrainSize and GSize is centimeter.

The grain size also can be scaled with the GrainFactor parameter:

```
pdbSet PolySilicon GrainFactor <n>
```

The default value of GrainFactor is 1.

### 3: Ion Implantation

#### Monte Carlo Implantation

The polycrystalline model works by frequently switching between the crystal algorithm and the amorphous algorithm. The probability of switching from the crystal model to the amorphous model is determined by the accumulative path length in crystal (`pathlength`) and polycrystalline grain size (`GrainSize`). It switches from the crystal model to the amorphous model if:

$$\text{pathlength} > R_{\text{rand}} \cdot (\text{GrainFactor} \cdot \text{GrainSize}) \quad (97)$$

where  $R_{\text{rand}}$  is a random number between 0 and 1. The polycrystalline model shares the same random number sequence with other modules in MC implantation. Therefore, if the random seed is reset, the random numbers used in the polycrystalline model are changed as well.

After an amorphous collision is processed, the `pathlength` is reset to zero, and the crystal model is selected. The `pathlength` is accumulated again. The model used for the next collision is again determined by the same rules. This process is repeated until the particle exits the polycrystalline region.

---

## Monte Carlo Implantation Into Alloy Materials

This section describes MC implantation into alloy materials.

### Defining Alloy Materials

In Sentaurus Process, a mole fraction-dependent alloy material is defined using a concentration field in a base material. For example,  $\text{Si}_{1-x}\text{Ge}_x$  is defined by either adding a germanium field in the base material silicon, or adding a silicon field in the base material germanium. As another example,  $\text{In}_{1-x}\text{Ga}_x\text{As}$  is defined by either adding a gallium field in the base material InAs, or adding an indium field in the base material GaAs.

In the previous scheme, the alloy material definitions are specified in the base material using `CompoundNumber`, `TernaryCompounds`, and `QuaternaryCompounds`. The mole fraction is calculated by dividing the field concentration by the lattice density of the base material.

In the more generalized scheme, the alloy materials are specified using the PDB parameters `Derived.Materials` in the base materials and `MoleFractionAtoms` in the compound materials.

For example, SiGe is defined as an alloy material by default with the following commands:

```
pdbSetString Si Derived.Materials {SiGe}  
pdbSetString Ge Derived.Materials {SiGe}  
pdbSetArray SiGe MoleFractionAtoms {x Ge}
```

III–V alloys, for example, can be defined using the following commands:

```

pdbSet GaAs Derived.Materials {InGaAs AlGaAs GaPAs}
pdbSet InAs Derived.Materials {InPAs InGaAs}
pdbSet InGaAs MoleFraction.Atoms {x Gallium} ;# In(1-x)Ga(x)As
pdbSet AlInGaAs MoleFraction.Atoms {x Aluminum y Indium} ;# Al(x)In(y)Ga(1-x-y)As

```

When group III or group V atoms are doped into a III–V material, and the atoms are a different species from the components of the material, the material is converted to the new III–V alloy with the component list, including the doping species if the doping concentration exceeds the minimum concentration Min.Conv.Conc. For example, when indium atoms are doped into a GaAs material region, GaAs is converted to InGaAs if InGaAs is one of the derived materials of GaAs, and the maximum concentration of indium atoms in the region exceeds the indium Min.Conv.Conc parameter value of InGaAs. The mole fraction is calculated with the interpolated lattice density.

In MC implantation, the lattice is constructed with the base material, with the lattice constants interpolated between the base materials with mole fraction, and each lattice site is assigned to a type of atom with a probability proportional to their mole fractions. Sentaurus MC considers the fact that each specific lattice site will be occupied with certain types of atom only. Therefore, the substitution of the lattice atoms occurs only for those atoms with the same Group number. The default group number for each type of atom is the same as that in the periodic table. To change the group number, for example, use:

```
pdbSet ImplantData Carbon Group 4
```

For example, in  $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ , Ge and C have the same group number (IV) as Si, so both of them can substitute silicon atoms in its lattice sites.

Another example is  $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{P}_y$ , where In and Ga belong to the same group number (III), and As and P belong to the same group number (V). Suppose Ga occupies site 0 and As occupies site 1 in zinc-blende structures, then In can only occupy site 0 and P can only occupy site 1, with the occupation probabilities proportional to their mole fractions.

## Interpolating Physical Parameters

To obtain consistent results with mole fractions from 0 to 1, all MC implantation-related parameters must be interpolated in mole fraction-dependent materials. These include:

- Material-related parameters: AmorpThreshold, d.sim, DebyeTemperature, LatticeConstant, and SurfaceDisorder
- Species-related parameters: amor.par, casc.amo, casc.dis, casc.sat, casc.sur, disp.thr, ibca.amo, ibca.dis, ibca.sat, ibca.sur, LSS.pre, nloc.exp, nloc.pre, sat.par, scr.par, and surv.rat

### 3: Ion Implantation

#### Monte Carlo Implantation

See [Alloy Materials and Parameter Interpolation on page 25](#).

---

## Monte Carlo Implantation Into Silicon Carbide

Sentaurus MC supports ion implantation into crystalline silicon carbide (`SiliconCarbide`) with a hexagonal lattice. The hexagonal system has four crystallographic axes: three  $a$ -axes ( $a_1, a_2, a_3$ ) forming a plane, and a  $c$ -axis that is normal to the plane. The crystallographic orientations (planes and directions) typically are described with four Miller indices  $\langle i j t k \rangle$ . In the hexagonal system, since the sum of the first three indices is zero ( $i + j + t = 0$ ), the third index ( $t$ ) is redundant and can be omitted. Therefore, when specifying crystal orientations in hexagonal SiC, only three Miller indices  $\langle i j k \rangle$  are used in Sentaurus Process commands, such as `init` and `mater`.

Silicon carbide exists in many different crystal structures, called polytypes. All polytypes have a hexagonal frame with a carbon atom situated above the center of a triangle of Si atoms and underneath a Si atom belonging to the next layer. The difference among the polytypes is the stacking sequence between the succeeding double layers of carbon and silicon atoms. For example, 2H-SiC, 4H-SiC, and 6H-SiC have the AB, ABCB, and ABCACB stacking sequence, respectively. On the other hand, 3C-SiC has an ABC stacking sequence and is the only form of SiC with a zinc-blende crystal lattice structure. The default polytype for SiC is 4H.

To change to a different polytype, use the `mater` command:

```
mater name=SiliconCarbide hexagonal polytype= 2H | 3C | 4H | 6H
```

**NOTE** The lattice constants, the mass density, and the Debye temperature may differ for different polytypes. For convenience, Tcl procedures (`set2HSiC`, `set3CSiC`, `set4HSiC`, and `set6HSiC`) are provided to set these parameters for different SiC polytypes.

The default principal wafer orientation is  $\langle 0001 \rangle$  in SiC. The default primary flat orientation is  $\langle 11\bar{2}0 \rangle$ . The wafer orientation (`wafer.orient`) and the flat orientation (`notch.direction`) can be changed using:

```
init wafer.orient= {<i> <j> <k>} notch.direction= {<i> <j> <k>}
```

However, these settings are superseded by those material-specific settings as set in the `mater` command:

```
mater name=SiC vertical.orient= {<i> <j> <k>} horizontal.orient= {<i> <j> <k>}
```

where `vertical.orient` specifies the wafer orientation, and `horizontal.orient` specifies the flat orientation.

**NOTE** While the SiC wafer orientation is mostly <0001>, the common primary flat orientation can be either <1 $\bar{1}$ 00> or <11 $\bar{2}$ 0>, depending on the manufacturer. The primary flat orientation must be set accordingly to predict the channeling behavior correctly for a given implantation angle.

A miscut of 3.5–8.5° typically exists in SiC (0001) wafers. Sentaurus MC implantation can take into account this wafer miscut by specifying `miscut.tilt` and `miscut.toward` in the `init` command:

- `miscut.tilt` is the angle by which the actual wafer normal is tilted with respect to `wafer.orient` (that is, the *c*-axis in the default wafer orientation) in the crystal coordinate system.
- `miscut.toward` specifies the direction *towards* which the wafer normal is tilted.

Generally, the crystal *c*-axis, the wafer normal, and the `miscut.toward` direction form fan-shaped angles with the wafer normal in between, that is, in the default wafer orientation, the projection of the wafer normal to the crystal plane, formed by the *a*1-axis and *a*2-axis, is the `miscut.toward` direction. By default, there is no wafer miscut, that is, `miscut.tilt=0`.

The following simple example illustrates how to perform an MC implantation in SiC with wafer miscut:

```
# Set up the structure
line x loc= 0.0 tag= oxtop spac= 0.001
line x loc= 0.0015 tag= top spac= 0.001
line x loc= 0.5 spac= 0.0025
line x loc= 2.0 tag= bottom spac= 0.01

region Oxide xlo= oxtop xhi= top
region SiliconCarbide xlo= top xhi= bottom

# Specify the wafer miscut
init miscut.tilt= 4 miscut.toward= {1 -1 0}

# Choose different polytype (default is 4H-SiC)
set 6H-SiC

# Perform the implantation
implant Aluminum energy= 60 dose= 1e13 tilt= 0 rot= 0 sentaurus.mc \
    particles= 10000 info= 2

# Save the result
struct tdr= sic
```

For details about the model and a comparison with experimental data for various implantation conditions, see [22].

---

## Recoil Implantation

Sentaurus MC implantation provides a general model for recoil implantation, such as an oxygen knock-on effect. Generally, recoil species are handled the same way as cascade atoms, except that no vacancies are created at the displaced sites, and the recoil species are not recorded as interstitials when they stop. Instead, a separate dataset is created for each recoil species.

The recoil species is specified in the material composition. For example, to simulate the oxygen knock-on effect, the following is defined in the parameter database:

```
Oxide -> Composition -> Component0 -> Name = Silicon  
Oxide -> Composition -> Component0 -> StWeight = 1  
  
Oxide -> Composition -> Component1 -> Name = Oxygen  
Oxide -> Composition -> Component1 -> StWeight = 2  
Oxide -> Composition -> Component1 -> Recoil = 1
```

To initiate oxygen recoil implantation, specify `recoils` in the `implant` command:

```
implant <species> energy=<n> dose=<n> recoils
```

The datasets `Oxygen_Implant` and `Oxygen` are created, which contain displaced oxygen distributions that can be used to analyze the oxygen knock-on effect.

---

## Plasma Implantation

Three-dimensional tri-gated devices (FinFETs) have been used at the 22 nm node and are expected to continue at and beyond the 16 nm node. Doping of FinFETs must be three dimensional, and conformal doping with plasma implantation is a promising approach. Likewise, doping of planar devices is challenging, and plasma implantation offers capabilities not available in beamline implantations.

To offer this simulation capability, Sentaurus Process provides a plasma implantation doping module that accurately reflects both the hardware and process signatures as well as the physical properties of the associated deposition, etching, sputtering, implantation, knock-on, defect creation, and annihilation processes.

This MC implantation module includes the following features:

- Perform alternating steps of deposition and MC implantation. Users can specify the number of steps.
- Deposition of material on the surface is performed isotropically (that is, constant growth rate over the surface). Users specify the thickness. A minimum thickness is imposed by

Sentaurus MC, which reduces the number of steps if necessary to prevent the deposition of a layer that is too thin. The deposited material must be defined as usual, and users must specify the material composition of the layer.

- Specification of multiple-ion incidents on the wafer. The ion species must be defined before implantation as usual, and some typical ion species used in plasma implantation will be predefined. You can specify the dose, the energy distribution, and the angular distribution of each ion species. The dose for each ion is applied evenly for each step.
- An empirical model for conformal doping, in which the level of conformity can be specified by users.
- In addition to computing the concentration of ions that penetrate through the deposited overlayer, the MC implantation module allows for atoms to be knocked out of the overlayer and into the wafer, and tracks the damage and amorphization as usual.

You must define the plasma source before implantation can be performed. To avoid overly complex syntax in the `implant` command, Sentaurus Process provides two ways to specify the plasma source: simple source and complex source.

## Simple Source

Assuming that the multiple ion species in plasma have the same energy and angle distributions, simply specify the multiple species as a list in the `implant` command (other parameters such as `dose`, `energy`, and `tilt` can be specified as for a typical implantation):

```
plasma.source= {<species1>=<n> <species2>=<n> <species3>=<n> ...}
```

where:

- `plasma.source` specifies a list of ion species to be implanted. These species must be predefined in `ImplantData` as usual.
- The number after each species is the fraction of the total dose (as specified by the `dose` parameter) for the given species.
- All these species will have the same `energy`, `tilt`, `en.stdev`, and `tilt.stdev` as specified.

## Complex Source

In more complex cases, different species can have different energies and angle distributions. In this case, each species can be specified with its own implantation parameters (`energy`, `tilt`, `en.stdev`, and `tilt.stdev`). So, for each species, define it with an `implant` command:

```
implant species=<species1> energy=<n> tilt=<n> en.stdev=<n> tilt.stdev=<n>
implant species=<species2> energy=<n> tilt=<n> en.stdev=<n> tilt.stdev=<n>
implant species=<species3> energy=<n> tilt=<n> en.stdev=<n> tilt.stdev=<n>
...
...
```

### 3: Ion Implantation

#### Monte Carlo Implantation

where <species1>, <species2>, <species3> must be predefined in `ImplantData` as usual. Only parameters that differ from the default values must be specified.

Then, you can perform the real implantation in the same way as in the simple source case:

```
implant plasma.source= {<species1>=<n> <species2>=<n> ...} dose=<n> energy=<n>
tilt=<n> en.stdev=<n> tilt.stdev=<n> ...
```

where:

- `plasma.source` specifies a list of ion species to be implanted. These species must be the same as those in previous `implant` commands.
- The regular implantation parameters (`dose`, `energy`, and so on) will be the default for those species that are not specified. Essentially, this syntax is consistent with that for the simple source and reduces to the simple source if no implantation parameters are specified for each individual species.

## Deposition of Material

To specify the deposition of material during implantation, use `plasma.deposit` in the `implant` command:

```
implant plasma.source= {<species1>=<n> <species2>=<n> ...}
plasma.deposit= {material=<c> thickness=<n> steps=<n>}
dose=<n> energy=<n> tilt=<n> ...
```

where:

- `material` is the name of the material to be deposited, which must be specified before the implantation.
- `thickness` is the total thickness of the deposit material.
- `steps` is the number of deposition steps.

The deposition and implantation are performed alternatively. If `plasma.deposit` is not specified, or `material` is not specified, or `thickness` is not specified (or is equal to zero), no deposition is performed.

Two PDB parameters are available to allow users to control the minimum deposition thickness:

```
 pdbSet MCImplant PLAD Min.Deposit.Thickness <n>
pdbSet MCImplant PLAD Min.Deposit.Thickness.3D <n>
```

The `Min.Deposit.Thickness` and `Min.Deposit.Thickness.3D` parameters control the minimum deposition thickness in two dimensions and three dimensions, respectively. The unit for these parameters is micrometer.

## Knock-on and Knock-off Effect

The MC implantation module simulates the dopant knock-on and knock-off effect by specifying recoils in the `implant` command. In addition, you must specify the recoil species to be simulated in material composition.

For example, assuming the deposited material is `BHx`, and `Atom0` is Boron, the following commands specify boron as a recoil species:

```
pdbSetString BHx Composition Atom0 Name Boron
pdbSetDouble BHx Composition Atom0 StWeight 1
pdbSetBoolean BHx Composition Atom0 Recoil 1
pdbSetString BHx Composition Atom1 Name Hydrogen
pdbSetDouble BHx Composition Atom1 StWeight <x>
```

## Conformal Doping

Conformal doping is an important characteristic in plasma implantation. However, due to the complexity of plasma dynamics that involves manybody long-range interactions, the exact mechanism for conformal doping in plasma implantation is not well understood. Physically, this may be possible if one of the following mechanisms or their combination occurs, for example, in a trench:

- The ions become ionized anywhere in the ambient (including inside the trenches) and start their acceleration towards the silicon surface.
- The ions scatter off other particles in the plasma/ambient (including inside the trenches) and change their direction.

To account for such effects, an empirical model has been developed that is compatible with the current plasma implantation. In this model, instead of launching all ions from above the device, as in standard implantation, some ions are launched along the device surface (that is, the solid–ambient interface). The fraction of ions launched along the surface can be specified using the `conformal.spec` argument in the `implant` command:

```
implant <species> energy=<n> dose=<n> sentaurus.mc \
conformal.spec= {
    [fraction=<n>] |
    [fraction.field=<c>] |
    [xdir= {x.location= {<n> <n> ...} fraction= {<n> <n> ...}}
     ydir= {x.location= {<n> <n> ...} fraction= {<n> <n> ...}}
     zdir= {x.location= {<n> <n> ...} fraction= {<n> <n> ...}} ] }
```

### 3: Ion Implantation

#### Monte Carlo Implantation

A spatial-dependent conformal ratio can be specified in any of the following (mutually exclusive) ways:

- Use `fraction=<n>` to specify a uniform conformal ratio, where `fraction` is a number between 0 and 1.0. For example, if `fraction=0`, you will obtain standard plasma implantation results. If `fraction=1`, you will obtain fully conformal doping.
- Use the `select` command to define a scalar conformal ratio field with a value ranging from 0 to 1. This field is then specified in `fraction.field`.
- Use piecewise linear functions `xdir`, `ydir`, and `zdir` to specify the depth-dependent conformal ratios.

`xdir`, `ydir`, and `zdir` specify conformal ratios for surface elements whose surface normals point in the x-, y-, or z-direction, respectively. If the surface normal of an element is not aligned with either the x-, y-, or z-direction, interpolation among different directions is performed. In two dimensions, only `xdir` and `ydir` are required. In three dimensions, `xdir`, `ydir`, and `zdir` are required.

Piecewise linear conformal ratios are specified using a pair of lists, `x.location={...}` and `fraction={...}` (`x.location` and `fraction` must have the same number of elements), where `x.location` is the x-coordinate (depth).

If the depth is outside the specified range, the closest fraction will be used.

## Other Plasma Implantation–Related Parameters and Procedures

Sentaurus Process provides a simple model for taking into account the energy and tilt angle distributions of the plasma source. Given the mean and the standard deviation of the implantation energy and tilt angles, Sentaurus MC implantation samples the given energy and tilt distributions for each implantation particle. After the implantation energy and the tilt angle are determined, the particle tracing is computed using a standard procedure.

In addition to the normal implantation parameters, such as energy and tilt, you can specify the standard deviation of the implantation energy (`en.stdev`) or the standard deviation of the tilt angle (`tilt.stdev`) or both. For example:

```
implant <species> plasma dose=<n> energy=<n> en.stdev=<n> tilt=<n>
tilt.stdev=<n> sentaurus.mc
```

where the implantation parameters `energy` and `tilt` are the mean energy and the mean tilt angle, respectively.

You also can specify the minimum energy that is allowed for implantation using the command:

```
pdbsSet MCImplant MinEnergyCutoff <n>
```

Energy below the minimum energy will be truncated. The default minimum energy is zero. In addition, you can specify the maximum energy that is allowed using the command:

```
pdbSet MCImplant MaxNumStdevCutoff <n>
```

Here, `MaxNumStdevCutoff` must be an integer (default is 5). The highest energy for a given implantation must not exceed the mean energy by the amount of `en.stdev x MaxNumStdevCutoff`. Energy higher than this number will be truncated.

## Energy Distributions

The energetic distribution of different molecular and atomic ions, after extraction from the plasma, is known to cover the range from zero to the maximum energy  $E_{\max}$ , which is equal to the product of the ion charge multiplied by the extraction voltage. Sentaurus Process allows easy selection and addition of various energy distribution models.

In addition to the default Gaussian distribution, Sentaurus Process implements an alternative Burenkov model [23]. In this model, the energy distribution, as presented by Tian *et al.* [24] as an integral number of particles having their energy in a given interval, can be written in a differential form as follows [23]:

$$f(E) = \frac{5}{6 \cdot E_{\max}} \cdot \left( \frac{E}{E_{\max}} \right)^{-1/6} \quad (98)$$

The energy distribution  $f(E)$  presented in Eq. 98 is normalized, that is, the integral over all possible energies of the extracted ions, ranging from 0 to  $E_{\max}$ , is equal to one. Burenkov *et al.* have shown that, by using the energy distribution given by Eq. 98, excellent agreement can be obtained between simulations and experiments for  $\text{BF}_3$  plasma implantation [23].

## Tilt Angle Distributions

Different tilt angle distributions are available in plasma implantation. You can select the tilt angle distribution model using:

```
pdbSet MCImplant PlasmaEnergyDistributionModel \
    {Gaussian | Gaussian.Solid.Angle | Gaussian.3D}
```

The default Gaussian model is:

$$f(\text{tilt}) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2}\left(\frac{\text{tilt}}{\sigma}\right)^2\right) \quad (99)$$

This is a first-order approximation in which the number of particles per solid angle has a sharp maximum at `tilt=0`. This may not be ideal in certain situations.

### 3: Ion Implantation

#### Monte Carlo Implantation

The Gaussian.Solid.Angle model is:

$$f(\text{tilt}) = \frac{\text{tilt}}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2}\left(\frac{\text{tilt}}{\sigma}\right)^2\right) \quad (100)$$

Here, the additional factor `tilt` considers that the solid angle corresponding to a tilt angle is proportional to the tilt angle. Note that the standard deviation ( $\sigma$ ) has a slightly different meaning from the regular Gaussian distribution, that is, only  $1-1/e = 63.2\%$  of ions will be in the interval  $[0, \sigma]$ .

For Gaussian.3D (suggested by Burenkov *et al.* [23]), you must add a random 3D vector, in which each component has a random Gaussian distribution to the vertical unit vector, and calculate the corresponding tilt angle. In this case, the knock-on process in the plasma may lead to additional ion energy that has a Gaussian distribution. Here again,  $\sigma$  has a different meaning from the standard Gaussian distribution, that is, only  $\sim 40\%$  of ions are within the interval  $[0, \sigma]$ .

To select a different energy distribution model, use:

```
pdbSet MCImplant PlasmaEnergyDistributionModel {Gaussian | Burenkov}
```

To provide maximum flexibility for energy and tilt angle distributions, you also can provide your own distributions by modifying the following Tcl procedures in `Plasma.tcl`:

```
Plasma::Energy_Distribution {energy stdev}
Plasma::Tilt_Distribution {mean stdev}
```

**NOTE** Sentaurus Process does not check the validity of these user-defined distributions. If you change these distributions, you must provide the correct distributions to ensure correct implantation results.

---

## Implantation Damage and Point-Defect Calculation

The damage in a Sentaurus MC implantation is computed either using the Kinchin–Pease formula [20] (default) or in full-cascade mode if `cascades` is specified in the `implant` command. For details about damage calculation, see [Damage Accumulation and Dynamic Annealing on page 123](#).

The calculation of the damage datasets for Sentaurus MC is consistent with analytic implantation. At the end of an implantation step, the damage for this step (`Damage_LastImp`) is added to the Damage profile using:

$$\text{Damage} += \text{MCDFactor} \cdot \text{Damage}_\text{LastImp} \quad (101)$$

where `+=` indicates that the total damage is the sum of the new damage and the existing damage. The default value for `MCDFactor` is 1 and can be changed in the `implant` command or in the parameter database:

```
implant <species> sentaurus.mc mc.dfactor=<n>
pdbSetDouble <material> <dopant> MCDFactor <n>
```

The accumulated damage is taken into account automatically for subsequent MC implantations, unless the `Damage` dataset is reset by the `diffuse` command.

## Point Defects: Elemental Materials

Point-defect profiles after an MC run can be generated from the ballistic dopant profile using the `plus.one` or `effective.plus.n` model, or from the ballistic vacancy (Frenkel pair) and recoil profiles using the `frenkel.pair` model.

The `plus.one` model is the default for all MC simulations. In this case, the ballistic dopant profile `<dopant>_LastImp` is used according to [Eq. 52, p. 92](#).

Interstitial and vacancy profiles also can be calculated using the ballistic vacancy dataset `Vac_LastImp` generated during an MC implantation run. The argument `defect.model` must be set to `frenkel.pair`:

```
implant <species> sentaurus.mc defect.model= frenkel.pair
```

Using the MC-specific factors `MCIFactor` and `MCVFactor`, the profiles are calculated according to:

$$\begin{aligned} \text{Int_Implant} &+= \text{MCIFactor} \cdot \text{Vac}_\text{LastImp} + \text{IFactor} \cdot <\text{dopant}>_\text{LastImp} \\ \text{Vac_Implant} &+= \text{MCVFactor} \cdot \text{Vac}_\text{LastImp} \end{aligned} \quad (102)$$

The default values for `IFactor`, `MCIFactor`, and `MCVFactor` are 1. These factors can be changed in the parameter database:

```
pdbSet <material> <dopant> IFactor <n>
pdbSet <material> <dopant> MCIFactor <n>
pdbSet <material> <dopant> MCVFactor <n>
```

or on the command line:

```
implant <species> sentaurus.mc ifactor=<n> mc.ifactor=<n> mc.vfactor=<n>
```

Setting `ifactor`, `mc.ifactor`, and `mc.vfactor` in the `implant` command overwrites the parameter database entries.

### 3: Ion Implantation

#### Monte Carlo Implantation

If cascades is enabled in MC implantation and the point-defect model is set to `frenkel.pair`, the interstitial and vacancy profiles are calculated using the concentration of the recoil and vacancy as calculated based on the physics model:

```
implant <species> sentaurus.mc cascades defect.model= frenkel.pair
```

In this case, the interstitial and vacancy densities increase according to:

$$\begin{aligned} \text{Int\_Implant} &+= <\text{recoil}>_{\text{LastImp}} + <\text{dopant}>_{\text{LastImp}} \\ \text{Vac\_Implant} &+= <\text{vacancy}>_{\text{LastImp}} \end{aligned} \quad (103)$$

## Point Defects: Multicomponent Materials

In multicomponent materials, such as SiC, the material is composed of different atom types. When an impurity is implanted into SiC, both silicon and carbon lattice atoms can be displaced, thereby forming silicon interstitials or carbon interstitials, and leaving behind silicon-site or carbon-site vacancies. Instead of classifying them together as interstitials or vacancies, as in silicon, Sentaurus Process provides a mechanism to distinguish different types of interstitial or vacancy.

To generate distinct types of point defect in multicomponent materials, you must switch on the `DistinctDefects` flag, for example:

```
pdbSetBoolean SiliconCarbide DistinctDefects 1
```

By default, this flag is true for SiC but false for other materials. As a result, instead of `Int_Implant` and `Vac_Implant`, the generated point-defect datasets in SiC are `IntSilicon_Implant`, `IntCarbon_Implant`, `VacSilicon_Implant`, and `VacCarbon_Implant`.

In this model, the total point-defect concentration is computed in the same way as for elemental materials. The implantation arguments `defect.model`, `ifactor`, `vfactor`, `mc.ifactor`, and `mc.vfactor` in the `implant` command still work:

- `ifactor` and `vfactor` are scaling factors for interstitial profiles and vacancy profiles, respectively, in the `plus.one` model.
- `mc.ifactor` and `mc.vfactor` are scaling factors for interstitial profiles and vacancy profiles, respectively, in the `frenkel.pair` model.

The same Tcl procedure `CalcPlusNFactor` calculates automatically the plus factors for the `effective.plus.n` model.

Then, the individual point-defect concentration is computed by multiplying the total point-defect concentration by a fraction of each component. The fraction of each component is, by default, its stoichiometric weight, but it can be changed in the parameter database with the parameters `IFactor.Fraction` and `VFactor.Fraction`. For example, in SiC:

```
pdbSet SiC Composition Component0 IFactor.Fraction <n>
pdbSet SiC Composition Component1 IFactor.Fraction <n>
pdbSet SiC Composition Component0 VFactor.Fraction <n>
pdbSet SiC Composition Component1 VFactor.Fraction <n>
```

If `cascades` is enabled in MC implantation and the point-defect model is set to `frenkel.pair`, the interstitial and vacancy profiles are calculated using the concentration of the recoils and vacancies as calculated based on the physical model.

In this case, the interstitial and vacancy densities increase according to:

$$\begin{aligned} \text{Int}<\text{component}>_{\text{Implant}} &+= <\text{component}>_{\text{LastImp}} + \text{IFactor.Fraction} \cdot <\text{dopant}>_{\text{LastImp}} \\ \text{Vac}<\text{component}>_{\text{Implant}} &+= <\text{vacancy-component}>_{\text{LastImp}} \end{aligned} \quad (104)$$

## Statistical Enhancement

The energetic pseudoparticles in an MC simulation are statistical objects representing several actual particles or only a fraction of an actual particle. Pseudoparticles start their motion at a plane above the target parallel to the wafer surface. The starting surface is subdivided into segments of equal size. The size of these segments is controlled by setting `dy` and `dz` in the `MCImplant -> Intervals` entry in the parameter database.

The number of pseudoparticles per segment (`dy` in two dimensions, and `dy x dz` in three dimensions) is set using:

```
pdbSet MCImplant Particles <n>
```

or:

```
implant <species> sentaurus.mc particles=<n>
```

The default value for `particles` is 1000. The random number generator can be started with a specified random seed. The integer value used can be set with `RandomSeed`:

```
pdbSet MCImplant RandomSeed <n>
```

The default is 1. Random seeds also can be chosen randomly by using the internal clock, thereby giving different results for different runs. This feature is useful for statistical analysis of MC implantations. To use this feature, specify:

```
pdbSet MCImplant Randomize 1
```

## Trajectory Splitting

Trajectory splitting artificially increases the number of trajectories in regions with low particle concentration. It can be switched on or off using:

```
pdbSet MCImplant TrajectorySplitting 1
```

When a particle is split, it is replaced by two *child* particles having half the statistical weight of the *parent* particle. At a split point, the two child projectiles start under identical conditions. Then, the trajectories of both child particles are simulated in the same way as for the original particle. However, consideration of thermal vibrations of target atoms leads to a deviation of the trajectories of the child projectiles after a few collisions. In this way, a high number of different particle trajectories with low statistical weight is obtained, which leads to an important decrease of the statistical noise in the tail parts of the dopant distribution.

Further splitting may occur that leads to a splitting tree related to the parent particle. The maximum depth of the splitting tree is defined by a global parameter `MaxSplitLevels`:

```
pdbSet MCImplant MaxSplitLevels <n>
```

In Sentaurus MC, you can chose the type of splitting model with the following command:

```
pdbSet MCImplant SplitModel {depth.sp | traj.density | coll.density}
```

- `depth.sp` (depth split) is the default model. It dynamically determines the splitting depths. If a particle reaches the splitting depth, it is replaced by two child particles, each with half the weight of the parent particle. A particle can be split multiple times if it reaches several splitting depths. This model maintains the same number of virtual particles at any depth, but their weights decrease with depth. The total number of virtual particles could be several times larger than the number of original particles. This model is very effective for reducing the noise in the tail portion of the profiles. However, it is less effective in improving the lateral statistics in 2D or 3D applications.
- `traj.density` (trajectory density) is a splitting model based on the trajectory density that has been accumulated in each volume element during the simulation. Trajectory density is the sum of the trajectory segments of all particles previously registered in the element divided by its volume. If a particle reaches an element with a small trajectory density from an element with a high trajectory density, a split point is set, that is, the particle is replaced by two child particles having half the statistical weight of the parent projectile. This splitting model is more effective in improving lateral statistics such as channels in 2D or 3D applications. However, it generally splits more particles and is slower than `depth.sp`.
- `coll.density` (collision density) is a splitting model based on the collision density. It splits the particles if the difference between two adjacent elements is sufficiently large. This model is less efficient and is deprecated.

## Dose Split

In the conventional pseudoparticle MC approach, all particles have the same weighting. In contrast, the dose split algorithm uses *smart* particle weighting with first-coming ions weighing less than later ions. This prevents crystalline from amorphizing too quickly, thereby allowing more ions to enter the channeling regions. This model can drastically reduce the noise of the channeling tails. By default, dose split is switched off. To activate the model, use the command:

```
pdbsSet MCImplant DoseSplit 1
```

The dose split model is especially effective for high-dose amorphizing implantations, such as arsenic implantation with a dose of  $8 \times 10^{15} \text{ cm}^{-2}$ . For a typical run, the CPU time is about 2 to 3 times slower than that without dose split for the same number of particles. However, dose split improves the statistics in the channeling tails by at least two orders of magnitude.

To achieve the same statistical significance, the conventional approach requires at least 100 times more particles; this means that the effective speedup is about 30 to 50 times.

## Trajectory Replication

The trajectory replication algorithm uses the fact that in almost all 2D or 3D target structures, several regions with 1D topology can be found. A particle trajectory going through such a part can be copied many times by shifting its origin. Within the 1D region, each shifted trajectory is a valid particle trajectory. Its reproduction by copying is much faster than its physical calculation.

The subdivision into 1D parts or *equivalence classes* is performed automatically during the implantation. A subdivision is performed using the segments of the start surface. At the beginning, all the start segments are in the same equivalence class.

First, the entire trajectory tree is calculated including splits and recoils. The increments of all concentration-type values, between entering and leaving a grid element, are stored for each trajectory point (at least one per grid element). A start segment is chosen from the same equivalence class. The starting point of the copy trajectory is set randomly within this start segment. The point where the copied trajectory enters the material is found in the same way as for the original trajectory. The vector between the first material point of the master trajectory and the copied trajectory serves as a shift vector. All increments of the master trajectory are transferred point-by-point into grid elements that correspond to the shifted points.

If the materials are not identical within geometric tolerance ( $1.5 \times 10^{-4} \mu\text{m}$ ), or the initial damage is different by more than 1% at the master and the replica points, replication fails and the start segment is taken out of the present equivalence class and placed into a new equivalence class. The generation of new equivalence classes ceases after a certain number of particles has been implanted. These initial particles are called *probing ions*.

### 3: Ion Implantation

#### Monte Carlo Implantation

Due to the random nature of ion trajectories, for the same structure, the equivalence classes as discovered by the probing ions could be slightly different depending on the random seeds, implanted species, or the number of probing ions.

The number of probing ions is set empirically to the total number of start segments. However, depending on the situation, this number may be too small for 2D simulations; whereas, it may be too large for 3D simulations. You can control this number using the command:

```
pdbSet MCImplant ReplicationLearningFactor <n>
```

After this command, the new number of probing ions will be equal to the original number of probing ions multiplied by `ReplicationLearningFactor`. Generally, the more probing ions, the more equivalence classes will be created for a given structure. More equivalence classes will reduce the ratio of the replicated trajectories to the calculated trajectories, thereby providing more accurate results at the expense of more CPU time.

The total number of implanted particles is given as the number of start segments multiplied by the number of particles per segment, which can be set using the parameter `particles`. Due to the replication, the number of physically calculated trajectories is usually much smaller and is given rather by the number of equivalence classes multiplied by `particles`.

When lateral straggling is greater than the length of the start segments, the trajectories replicated in neighboring segments may overlap significantly. This overlap may result in reduced simulation accuracy because, essentially, the damage effect between these trajectories is ignored (physically, the damage will cause different trajectories since the initial trajectories create damage and the subsequent trajectories see the damage). To preserve the accuracy, the length of the start segment `dy` or `dz` must be at least a few times larger than the lateral straggling. The defaults `dy=0.05 μm` and `dz=0.05 μm` are reasonable choices for low-to-medium energy implantations. However, for high-energy implantations, the lateral straggling can be quite large. Therefore, you may need to increase `dy` and `dz`. In the worst case, `dy` and `dz` may be so large (especially for high-energy implantations) that they cover the entire lateral dimension of the device. In this case, no replication can be performed, thereby reducing the simulation performance.

Smaller values of `dy` and `dz` result in a higher replication ratio and, therefore, better performance. However, smaller values can cause significant trajectory overlap, thereby degrading simulation quality. To preserve the accuracy of the simulation with trajectory replication, it is crucial to be able to choose `dy` and `dz` automatically. This can be achieved by launching a 1D simulation to precompute the lateral straggling.

To enable automatic values for `dy` and `dz`, use the following commands:

```
pdbSet MCImplant Auto.Dy.Dz 1  
pdbSet MCImplant Dy.Dz.Factor <n>
```

The default of `Dy.Dz.Factor` is 2.0. Assuming that the calculated straggling by 1D MC implantation is  $\sigma$ , `dy` and `dz` are determined by the following formula:

$$dy = dz = Dy.Dz.Factor \cdot \sigma \quad (105)$$

The trajectory replication algorithm is based on the heuristic argument that the 1D part of the structure should be equivalent. However, some parts of the 1D region may be close to the sidewalls. Therefore, the dopant concentration is contributed to not only from the direct exposure to the ion beam, but also from the particles scattered from the sidewalls and re-entering the 1D region. In such situations (such as high-energy implantation into a photoresist mask or pocket implantations), trajectory replication may not give accurate results near the sidewalls. In addition, for high-tilt pocket implantations, saving CPU time by trajectory replication is limited. Therefore, under such circumstances, you should switch off trajectory replication.

**NOTE** Trajectory replication is switched on by default. To switch off trajectory replication, use the global switch:

```
pdbSet MCImplant TrajectoryReplication 0
```

## Datasets

The datasets used in an MC run follow the same naming conventions as those used in analytic implantation. Datasets unique to the MC implantation method are:

- The ballistic vacancy density `Vac_LastImp`.
- The nuclear energy deposition `EnergyDeposition`.

Table 10 Datasets used in Monte Carlo implantations

Dataset	Description
<code>Damage</code>	Accumulative damage (damage history). At the end of an implantation step, the <code>Damage_LastImp</code> concentration is added to <code>Damage</code> , similar to analytic implantation. The <code>diffuse</code> command deletes this dataset.
<code>Damage_LastImp</code>	Damage created during the last implantation step.
<code>&lt;dopant&gt;</code>	Accumulative density of the dopant concentration. At the end of an implantation step, the <code>&lt;dopant&gt;_LastImp</code> concentration is added to <code>&lt;dopant&gt;</code> .
<code>&lt;dopant&gt;_Implant</code>	Accumulative density of the dopant concentration. At the end of an implantation step, the <code>&lt;dopant&gt;_LastImp</code> concentration is added to <code>&lt;dopant&gt;_Implant</code> . The <code>diffuse</code> command deletes this dataset.
<code>&lt;dopant&gt;_LastImp</code>	Ballistic dopant concentration generated during the last implantation step. It is reset at the beginning of each implantation step.
<code>EnergyDeposition</code>	Accumulated energy deposition (in units of eV/cm <sup>3</sup> ) from nuclear collisions.

### 3: Ion Implantation

#### Monte Carlo Implantation

Table 10 Datasets used in Monte Carlo implantations

Dataset	Description
Int_Implant	Accumulative interstitial profile updated at the end of an implantation step.
Int<component>_Implant	Accumulative interstitial profiles in multicomponent material with <code>DistinctDefects</code> set to true, where <component> is the component of the composition of the material. For example, in SiC, interstitial profiles include IntSilicon_Implant and IntCarbon_Implant.
Vac_Implant	Accumulative vacancy profile updated at the end of an implantation step.
Vac_LastImp	Ballistic vacancy density generated during the last implantation step.
Vac<component>_Implant	Accumulative vacancy profiles in multicomponent material with <code>DistinctDefects</code> set to true, where <component> is the component of the composition of the material. For example, in SiC, vacancy profiles include VacSilicon_Implant and VacCarbon_Implant.

---

## Multithreaded Parallelization of Sentaurus MC Implantation

The performance of Sentaurus MC can be significantly improved by using multithreaded parallelization. In this approach, a large job with many particles ( $N$ ) is divided into multiple ( $m$ ) separate jobs with a smaller number of particles ( $N/m$ ). Sentaurus Process then creates multiple threads and launches  $m$  instances of Sentaurus MC implantation. Each instance of Sentaurus MC implantation runs independently on its own thread. After these threads are finished, the results are averaged, thereby improving the effective execution speed for a large job.

To engage the multithreaded parallelization of Sentaurus MC implantation, use the `math` command (see [math on page 1073](#)):

```
math numThreads=<i> | numThreadsMC=<i>
```

where `numThreads` is a general keyword for MC implantation and 3D analytic implantation. However, `numThreadsMC` has higher priority over `numThreads` for Sentaurus MC implantations and can be used to create the number of threads specifically for Sentaurus MC implantation, which is different from that for other multithreaded operations. The value of `numThreads` or `numThreadsMC` must equal the number of cores in multicore processors.

You also can modify the stack size for each thread using the command:

```
math threadStackSize=<i>
```

The default stack size ( $2^{18} = 262144$  bytes) is usually sufficient for Sentaurus MC implantation.

---

## Boundary Conditions and Domain Extension

Boundary conditions are needed in ion implantations to account for geometric effects (such as shadowing) and lateral scattering of the implied structure. Both these effects require knowledge of the materials and damage concentration outside the simulation domain. The required information is synthesized by the definition of the boundary conditions. This section describes how to specify these boundary conditions.

---

### Unified Implantation Boundary Conditions

**NOTE** This is the preferred method for specifying implantation boundary conditions.

Sentaurus Process has two different sets of implantation boundary conditions: one for analytic implantation and one for MC implantation. To ensure consistent results between analytic and MC implantations, Sentaurus Process provides a unified method for specifying implantation boundary conditions. This method uses the `implant` command to specify the boundary conditions with the following syntax:

```
implant boundary.conditions= {left=<c> right=<c> front=<c> back=<c>}
```

where the valid options are `Periodic`, `Reflect`, or `Extend`.

In contrast to the boundary conditions specified by PDB commands, if `Periodic` or `Reflect` is specified in the `implant` command, `TruePeriodic` and `TrueReflect` will be used for MC implantation since these ensure the most consistent results between analytic and MC implantations.

You do not need to specify boundary conditions for all four sides. The `Extend` boundary condition is assumed for unspecified sides, except for periodic boundary conditions. Since periodic boundary conditions must be paired (left and right, or front and back), they must have the same periodic boundary conditions. For simplicity, you need only specify periodic boundary conditions on one side; the other side is assumed automatically to have the same periodic boundary condition. If the other side is specified for a different type of boundary condition, Sentaurus Process issues a warning and uses periodic boundary conditions.

---

### Implantation Boundary Conditions Using PDB Commands

**NOTE** This method for specifying implantation boundary conditions is obsolete. Do not use this method when creating new command files.

### **3: Ion Implantation**

#### Boundary Conditions and Domain Extension

Boundary conditions can be specified directly using PDB commands. Advanced users can use these commands to adjust the implantation boundary conditions under certain circumstances.

## Monte Carlo Implantation

Boundary conditions determine how particles leaving the simulation domain at its outer boundaries will be processed.

It is assumed that the simulation domain is rectangular if viewed from the top and is contained between:

`LeftBoundary` and `RightBoundary` (y-direction)

and:

`BackBoundary` and `FrontBoundary` (z-direction)

### **TruePeriodic Boundary Conditions**

These boundary conditions consider the device to be a true periodic structure. To select `TruePeriodic` boundary conditions, use:

```
pdbSet MCImplant TruePeriodicY 1  
pdbSet MCImplant TruePeriodicZ 1
```

Here, `TruePeriodicY` and `TruePeriodicZ` are applied to the left and right, and to the front and back, respectively.

**NOTE** The `TruePeriodic` boundary conditions take precedence over legacy periodic boundary conditions and other types of boundary condition. If `Periodic` is specified in the `implant` command for unified implantation boundary conditions, `TruePeriodic` boundary conditions are selected automatically for MC implantation.

### **Legacy Periodic Boundary Conditions**

**NOTE** These boundary conditions are obsolete. Do not use them when creating new command files.

In this boundary condition, boundaries exist only in solid regions. In solid regions, when a particle reaches one side of the boundary, it is moved to the other side of the boundary. However, in ambient (or gas), particles are free to enter or exit. Therefore, the periodic boundary conditions in MC implantation only mean translating the position of particles from one boundary to the opposite boundary in solid regions. It takes the structure as it is and does not extend to form a true periodic structure.

To select these boundary conditions, use the following commands:

```
 pdbSet MCImplant BoundaryPeriodicY 1  
 pdbSet MCImplant BoundaryPeriodicZ 1
```

This switches on periodic boundary conditions in the left-right and front-back, respectively.

### TrueReflect Boundary Conditions

Instead of reflecting the direction of the moving particles at the boundary, Sentaurus Process provides TrueReflect boundary conditions that automatically reflect the structure, perform the implantation, and then cut the structure to its original domain. To specify TrueReflect boundary conditions, use:

```
 pdbSet MCImplant LeftBoundary TrueReflect  
 pdbSet MCImplant RightBoundary TrueReflect  
 pdbSet MCImplant FrontBoundary TrueReflect  
 pdbSet MCImplant BackBoundary TrueReflect
```

**NOTE** If Reflect is specified in the implant command for unified implantation boundary conditions, TrueReflect boundary conditions are selected automatically in MC implantation.

**NOTE** Generally, reflective boundary conditions (including both Reflect and TrueReflect) can be used only if there are the same reflect-symmetric ion beams, such as tilt=0 (or projected tilt2D=0 in two dimensions), or approximately, multiple rotation implantations. To improve performance, averaging of the simulation results (including dopant and damage fields) over the original and reflected domains can be performed. If tilt (or tilt2D) < 2°, Sentaurus Process automatically averages the simulation results. In the case of multiple rotation (mult.rot) implantations (or a sequence of multiple implant commands consisting of multirotation implantation), no automatic averaging is performed. However, you can specify average in the implant command to perform the averaging. To overwrite such default behaviors, specify average or !average in the implant command.

**NOTE** In cases where average is applied successfully, TrueReflect generally achieves more accurate results than Reflect without the significant performance penalty.

### 3: Ion Implantation

#### Boundary Conditions and Domain Extension

### Legacy Reflect Boundary Conditions

A particle hitting the boundary will have its position and direction of motion reflected with respect to the boundary plane:

```
pdbSet MCImplant LeftBoundary Reflect  
pdbSet MCImplant RightBoundary Reflect  
pdbSet MCImplant FrontBoundary Reflect  
pdbSet MCImplant BackBoundary Reflect
```

### Extending the Simulation Domain

The simulation domain is extended artificially in the corresponding direction:

```
pdbSet MCImplant LeftBoundary Extend  
pdbSet MCImplant RightBoundary Extend  
pdbSet MCImplant BackBoundary Extend  
pdbSet MCImplant FrontBoundary Extend
```

This compensates for the decay of the profile near the boundaries of the simulation domain. Sentaurus Process determines these extension lengths automatically by using `tilt`, `rotation`, and `slice.angle`, and the user-defined parameters `MinExtension` and `ExtensionLength`:

$$\text{Extension Length} = \text{MinExtension} + \text{ExtensionLength} \cdot f(\text{tilt}, \text{rotation}, \text{slice.angle}) \quad (106)$$

where the function  $f$  is between 0 and 1. If `tilt=0`,  $f$  equals 0. Therefore, for `tilt=0`, the extension length equals `MinExtension`. The default value for `MinExtension` is  $0.1 \mu\text{m}$ , which is usually sufficient for low-energy implantations. For high-energy implantations, you may need to increase `MinExtension` to avoid decaying concentration near the boundaries.

To control the size of the extension, use:

```
pdbSet MCImplant ExtensionLength <n>  
pdbSet MCImplant MinExtension <n>
```

### Transparent Boundary

All particles crossing the boundary leave the simulation domain and are lost:

```
pdbSet MCImplant LeftBoundary Transparent  
pdbSet MCImplant RightBoundary Transparent  
pdbSet MCImplant BackBoundary Transparent  
pdbSet MCImplant FrontBoundary Transparent
```

**NOTE** For given boundary conditions other than Transparent, it is important that the boundaries, which are lines in two dimensions and planes in three dimensions, are continuous, that is, they should show no holes. The crossing of a particle can only be registered if it happens within the material region. The particle will finally leave the structure if it crosses the side while in a gas region.

## Analytic Implantation

Analytic implantation uses the same syntax as MC implantation for specifying boundary conditions. It is assumed that the simulation domain is rectangular if viewed from the top and is contained between:

`LeftBoundary and RightBoundary (y-direction)`

and:

`BackBoundary and FrontBoundary (z-direction)`

## Extended Boundary Conditions

The simulation domain is extended artificially in the corresponding direction:

```
pdbSet ImplantData LeftBoundary Extend  
pdbSet ImplantData RightBoundary Extend  
pdbSet ImplantData FrontBoundary Extend  
pdbSet ImplantData BackBoundary Extend
```

This compensates for the decay of the profile near the boundaries of the simulation domain. The extended structure is removed after the implantation is completed. `Extend` is the default boundary condition for ion implantation. To control the size of the lateral extension, use:

```
pdbSet ImplantData MaxLateralExtension <n>
```

## Reflective Boundary Conditions

In reflective boundary conditions, a reflected image with respect to the domain boundary is first constructed:

```
pdbSet ImplantData LeftBoundary Reflect  
pdbSet ImplantData RightBoundary Reflect  
pdbSet ImplantData BackBoundary Reflect  
pdbSet ImplantData FrontBoundary Reflect
```

Depending on the boundary condition specified on the other side, the composite structure is either extended (if the other side is extended) or repeated (if the other side is also reflective).

### 3: Ion Implantation

#### Smoothing Implantation Profiles

The added structure including the reflected image is removed after the implantation is completed.

**NOTE** These boundary conditions are equivalent to `TrueReflect` boundary conditions in MC implantation.

#### Periodic Boundary Conditions

These commands switch the periodicity in the left-right or front-back direction, respectively:

```
pdbSet ImplantData BoundaryPeriodicY 1  
pdbSet ImplantData BoundaryPeriodicZ 1
```

An array of periodic images is constructed outside the simulation domain before the implantation is performed. These added periodic images are removed after the implantation is finished.

**NOTE** These boundary conditions are equivalent to `TruePeriodic` boundary conditions in MC implantation.

---

## Smoothing Implantation Profiles

The implantation profiles produced by MC simulations are typically noisy, especially in low concentration regions. This may cause convergence problems or may require a very small time step in diffusion. To overcome this problem, Sentaurus Process provides a facility for smoothing the implantation profiles.

The smoothing is enabled by using a simple diffusion equation:

$$\frac{\partial C}{\partial t} - (D \cdot \nabla C) = 0 \quad (107)$$

where:

- $C$  is the concentration.
- $D$  is the diffusion coefficient.
- $\sqrt{D \cdot t}$  is the characteristic diffusing distance.

---

## Smoothing All As-Implanted Profiles

To smooth all as-implanted profiles, specify `smooth` in the `implant` command, or use the global switch `Smoothing`, for example:

```
pdbSet MCImplant Smoothing 1
```

In this case, all as-implanted fields are smoothed including dopant, damage, and point-defect profiles.

---

## Smoothing Dopant and Damage Fields

For flexibility, Sentaurus Process provides facilities to smooth selected fields using `smooth.field= <list>` in the `implant` command. If `smooth.field` is specified, only the specified fields are smoothed. The valid fields are `<dopant>` or `Damage`. For example, for  $\text{BF}_2$  implantation, the valid fields are `Boron`, `Fluorine`, or `Damage`. Note that point defects (interstitial and vacancy) are generally not independent and cannot be specified in `smooth.field`. In addition, depending on the point-defect model used, the smoothing of dopant or damage fields also may cause the point defects to be smoothed.

To control smoothing behavior, specify `smooth.distance= {<double array>}`. This list specifies the smoothing distances (diffusing distance) for each of the fields as specified in `smooth.field`. If this list is missing, the smoothing distances are retrieved from the PDB:

```
pdbSetDouble MCImplant Smooth <dopant> Smooth.Distance <n>
```

If no `pdb` parameter is available for a given species, the global default (2 nm) is used.

---

## Smoothing Point Defects

If only point defects are smoothed, you must use the `smooth` command after the `implant` command (instead of specifying `smooth` or `smooth.field` in the `implant` command). The syntax is:

```
smooth smooth.field= <list> smooth.distance= {<double array>}
```

This is a general command that can be used to smooth any field. For example, to smooth point defects after implantation, use:

```
smooth smooth.field= {Int_Implant Vac_Implant} smooth.distance= {1<nm> 5<nm>}
```

### 3: Ion Implantation

#### Automatically Extracting Implantation Moments

**NOTE** If you use the `smooth` command to smooth a field, the `pdb` parameter `Smooth.Distance` will not be read. Therefore, `smooth.distance` must be specified in the `smooth` command if it differs from the default 2 nm.

---

## Automatically Extracting Implantation Moments

Implantation moments are one of the most critical elements in analytic implantation. By default, Sentaurus Process provides a large set of implantation tables that cover many species and materials, and a wide range of implantation conditions. However, occasionally, you may want to explore new species, new materials, or the implantation parameter space, which is outside of the supplied implantation tables. In this case, you need to perform experiments or to run MC implantation simulations to obtain accurate implantation profiles. Automatically extracting implantation moments bridges the gap of converting these raw profiles into the moments that can be used in analytic implantation.

The critical part of automatic extraction of implantation moments is the optimization (or least-square fit) algorithm, that is, given a profile or a set of  $m$  pairs of data points  $(x_i, y_i)$ , you optimize the parameter set  $\beta$  of the model function  $f(x, \beta)$ , so that the sum of the squares of the errors at each point becomes minimal:

$$S(\beta) = \sum_{i=1}^m [y_i - f(x_i, \beta)]^2 \quad (108)$$

Sentaurus Process uses the same optimizer as TSUPREM-4, which implements the popular Levenberg–Marquardt algorithm, also known as the damped least-squares method. Since this algorithm only finds the local minimum, the initial parameter values may affect the extracted results.

---

## Required Parameters

To extract the moments, you must specify `extract.moments` and `data.file` in the `implant` command:

- `extract.moments` simply indicates that instead of performing an implantation or setting implantation parameters, the `implant` command is used to extract implantation moments.
- `data.file` specifies the ASCII data file from where implantation moments will be extracted.

## Optional Parameters

To better control the extraction process, the following optional parameters are available in the `implant` command:

- `dualpearson` (default), `gaussian`, and `pearson` specify the type of moments to be extracted.
- `rp`, `stdev`, `gamma`, `beta`, `rp2`, `stdev2`, `gamma2`, `beta2`, and `ratio` specify the initial values for optimization. If not specified, initial values will be guessed from the profile data.
- `data.units`, `data.xcol`, `data.col`, `data.xlo`, `data.xhi`, `data.min`, and `data.max` specify how the data in `data.file` will be interpreted and retrieved.
- `max.iter` specifies the maximum number of iterations allowed in the optimization loop. Default is 500.
- `tolerance` specifies the tolerance of target errors. Default is 0.1.

## Output Format

Extracting implantation moments provides two types of output, at the same time, to facilitate further manipulation of the moments:

- Command line. This is useful for copying and inserting the output into the `implant` command. The extracted moments are printed on the screen and in the log file in the format:  
`rp=<n> stdev=<n> gamma=<n> beta=<n> ...`
- Tcl list. The output list of moments has the format:

```
{model dualpearson rp <n> stdev <n> gamma <n> beta <n> ... rms <n>}
```

The output Tcl list can be converted into a Tcl array using `array set`, which then can be used to access the moments conveniently, for example:

```
set moms [implant extract.moments data.file=myfile]
array set m $moms
LogFile "'model = $m(model) ''"
LogFile "'rp = $m(rp) ''"
LogFile "'stdev = $m(stdev) ''"
LogFile "'rms = $m(rms) ''"
```

The root mean square (RMS) error is an important gauge for the fitting accuracy. Generally, if the RMS error is less than 1, the fitting looks very good visually.

### **3: Ion Implantation**

Automatically Extracting Implantation Moments

---

## **Utilities**

The Tcl script `ImplantTableMaker` can be used to guide users through selecting implantation conditions to automatically create a Taurus-formatted implantation table from MC implantations. You must first input various implantation parameters that are necessary to create an implantation table.

The resulting table is named `<species>_in_<material>_mystandard`.

This script can be run in either interactive mode or batch mode. To use this script, start Sentaurus Process:

```
% sprocess
```

Sentaurus Process enters interactive mode.

At the prompt, invoke `ImplantTableMaker` with or without a file name:

```
sprocess> ImplantTableMaker <filename>
```

If a file name is not specified, the default file name `ImplantTableMaker.in` is used. If the file does not exist, the script will create a file, enter interactive mode, and save user inputs into the newly created file. If the file exists, the script will enter batch mode and read the parameters from the file.

### **Interactive Mode**

In interactive mode, you will be asked to input the control parameters and the implantation conditions. All the control parameters have default values. Either press the Enter key to accept the default values or enter new values. The accepted values are shown on the screen.

The implantation conditions include the implantation species, the range of implantation energy, the dose, the tilt, the rotation angles, and the screen oxide thicknesses. These can be entered by a set of values separated by space or commas (,). The accepted values are shown on the screen.

User inputs are recorded in a text file. The file name is specified as an argument when you invokes `ImplantTableMaker`. If a file name is not specified when invoking `ImplantTableMaker`, a default file named `ImplantTableMaker.in` will be created. This file can be edited and then read by `ImplantTableMaker`, so that you do not need to enter the same information every time `ImplantTableMaker` is run.

**NOTE** If you do not specify a file name when invoking `ImplantTableMaker` and `ImplantTableMaker.in` exists in the current directory, Sentaurus Process will enter batch mode and read the information contained in the `ImplantTableMaker.in` file instead of entering interactive mode and requesting user information.

## Batch Mode

If the `ImplantTableMaker.in` file or a user-specified file exists, `ImplantTableMaker` will enter batch mode. In this mode, `ImplantTableMaker` will read the control parameters and the implantation conditions from the text file. This text file contains many lines with the format of a keyword and value pair. The following keywords are accepted:

- `particles`: The number of particles for the initial (first iteration of the) MC simulation.
- `particles.multiplier`: The multiplier of the particle number for the next iteration of the MC simulation if the previous extraction does not converge.
- `max.rms`: The maximum RMS error for acceptable fitting. Generally, the smaller the value, the better the fitting. A value of `rms=1.0` is recommended.
- `max.iterations`: The maximum number of iterations of MC implantation simulations if the previous extractions do not converge, that is, `rms > max.rms` for the previous iterations. If after `max.iterations`, the extraction still does not converge, a warning message is displayed, and manual extraction may be needed. If `max.iterations` is set to a very high value, in theory, the implantation table will be completed without any user intervention. However, it may take a very long CPU time to complete.
- `max.dynamic.range`: The maximum dynamic range is the range from the peak concentration to the minimum concentration that is taken into account in the extraction. Below the minimum concentration, the data points will be discarded for the purpose of extraction. This avoids any problems caused by profile noise. Typically, `max.dynamic.range` is `1e4` or `1e5`.
- `lat.stdev.factor`: Specifies `lat.stdev` as a fraction of the vertical `stdev` for the first Pearson, that is, `lat.stdev = lat.stdev.factor*stdev`.
- `lat.stdev2.factor`: Specifies `lat.stdev2` as a fraction of the vertical `stdev` for the second Pearson, that is, `lat.stdev2 = lat.stdev2.factor*stdev2`.
- `smooth`: Specifies whether smoothing is performed in the MC implantation. The accepted value is either 0 or 1.
- `AdvancedCalibration`: Specifies the Advanced Calibration version. The default is off.
- `species`: Specifies the implantation species.
- `material`: Specifies the material into which implantation is performed.
- `energies`: Specifies the energy range for the table using a list of discrete values.
- `doses`: Specifies the dose range for the table using a list of discrete values.
- `tilts`: Specifies the range of the implantation tilt angles using a list of discrete values.

### 3: Ion Implantation

#### Automatically Extracting Implantation Moments

- **rotations:** Specifies the range of rotation angles using a list of discrete values.
- **screens:** Specifies the screen oxide thicknesses using a list of discrete values. The unit is micrometer.

**NOTE** In batch mode, you can create a Sentaurus Process command file (for example, `maker.fps`), which contains one line (`ImplantTableMaker <filename>`), and then run Sentaurus Process as usual:

```
% sprocess maker.fps
```

### Example of Batch File for ImplantTableMaker Script

The following is an example of an `ImplantTableMaker.in` file. Note that each line consists of a keyword and a list of values separate by space or commas. This file is generated automatically in interactive mode, and can be edited and used in batch mode:

```
particles: 10000
max.rms: 1.0
max.iterations: 5
max.dynamic.range: 1e5
lat.stdev.factor: 1.0
lat.stdev2.factor: 0.6
smooth: 1
AdvancedCalibration: off
species: Boron
material: Silicon
energies: 1, 10, 100
doses: 1e13, 1e14, 1e15
tilts: 0, 7, 15, 30
rotations: 0, 10, 20, 30
screens: 0.0015
```

**NOTE** Since each implantation profile is extracted independently, and the Levenberg–Marquardt optimization algorithm can only find the local minima, slightly different profiles may result in totally different implantation moments. Interpolation between these moments may not give optimal results. Therefore, when using the Tcl script `ImplantTableMaker`, the quality of implantation tables cannot be guaranteed.

---

## Loading External Profiles

This section describes how to load external profiles.

---

### Loading External Profiles Using `load.mc` Switch

A precomputed external profile can be loaded in to a given structure using `load.mc`:

```
implant <species> energy=<n> dose=<n> tilt=<n> rotation=<n> load.mc file=<c>
```

If you use `load.mc`, you must also use the `file` argument to specify the TDR file to load. Sentaurus Process takes the TDR file specified and loads the datasets into the present structure. Interpolation of the datasets is performed if the structure in the TDR file differs from the present structure.

Sentaurus Process attempts to find the doping profiles required from the implantation species and the damage dataset. For example, in the following command, Sentaurus Process opens the file `my_data{_fps}.tdr` and checks for the `Boron_LastImp` and `Damage_LastImp` datasets:

```
implant Boron load.mc file= my_data energy= 10 dose= 1e14
```

If successful, these datasets are restored. If one or more of the required datasets is missing, the respective fields remain empty. Then, during implantation postprocessing, `Boron_LastImp` and `Damage_LastImp` are added to the `Boron_Implant` and `Damage` datasets.

When using `load.mc`, the following options are available for 2D structures:

- `shift=<n>`: Shifts the dataset along the y-axis.
- `flip`: Flips the dataset to the left.
- `left, right`: Specifies the flipping direction.
- `multiply=<n>`: Multiplies the dopant data in the dataset by a factor; the damage remains untouched.

**NOTE** The `load.mc` switch restores the datasets from the files without checking the implantation conditions specified in the `implant` command. Therefore, `load.mc` by itself does not require implantation parameters such as `energy` and `dose` to be specified. However, the CoImplant model may use these parameters (`energy` and `dose`) for its calculations. Therefore, it is recommended that `energy` and `dose` are always specified along with `load.mc`.

---

## Automated Monte Carlo Implantation

If no TDR file with the specified name is found or `file` is omitted, a separate run of Sentaurus MC is started to generate these files and the required datasets. Sentaurus Process internally switches from the `load.mc` mode to the `sentaurus.mc` mode. All implantation parameters related to MC implantation (`particles`, `cascades`, `full.molecular`) are used in this run.

**NOTE** The `load.mc` switch is designed to reuse precomputed MC results. However, the profiles to load do not necessarily need to be generated using the MC method.

### Example

```
implant BF2 dose= 1e14 energy= 40 tilt= 20 rotations= -90 load.mc \
    file= bf2_1e14_40 particles= 500 cascades
```

In the first run of this command, Sentaurus Process checks for the TDR file named `bf2_1e14_40`. Since there is no file with this name, a full-cascade Sentaurus MC run is started using the parameters specified. At the end, the TDR file `bf2_1e14_40_fps.tdr` is saved. The following are stored as well:

- All datasets related to the  $\text{BF}_2$  impurity profile (`Boron_LastImp`, `Fluorine_LastImp`).
- The damage (`Damage_LastImp`).
- The recoil profile (`Silicon_LastImp`) and the vacancy profile (`Vac_LastImp`) because the command is run in full-cascade mode.

In a subsequent run of the same command, Sentaurus Process loads and restores these datasets in a preprocessing step. The postprocessing is the same as after a MC run.

---

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*This chapter discusses the continuum models for dopant and defect diffusion models and parameters. For an atomistic approach, see [Chapter 5](#).*

---

## Overview

During the fabrication process, dopants are introduced into the substrate with different concentration profiles. As processing proceeds through various thermal annealing cycles, dopants diffuse and redistribute through the structure. The following effects contribute to dopant redistribution and can be modeled by Sentaurus Process:

- Dopant (de)activation
- Dopant–defect interaction
- Chemical reactions at interfaces and in bulk materials
- Material flow
- Moving material interfaces
- Internal electric fields

Sentaurus Process is designed to address the challenges of integrated-circuit process modeling. As technology development continues, the need for new process models increases. The Alagator language is a versatile way to add and modify diffusion models quickly. This chapter describes the diffusion models in Sentaurus Process. To modify or add new diffusion models, see [Modifying Built-in Equations and Terms on page 615](#).

The `diffuse` command represents the main simulation capabilities of Sentaurus Process and simulates:

- Thermal annealing of impurities.
- Material growth processes during annealing, for example, oxidation, silicidation, and epitaxy (see [Epitaxy on page 267](#) and [Oxidation on page 645](#)).
- Process-induced stress (see [Chapter 10 on page 677](#)).

---

## Basic Diffusion

The `diffuse` command is used to model the diffusion of impurities under oxidizing and non-oxidizing conditions. The arguments of the `diffuse` command set the diffusion conditions as well as time-stepping options (see [diffuse on page 935](#)). For example, a command for a simple non-oxidizing annealing at a temperature of 900°C for 10 s is:

```
diffuse temperature= 900<C> time= 10<s>
```

To perform the same anneal with a wet (H<sub>2</sub>O) oxidizing ambient, use the following command:

```
diffuse temperature= 900<C> time= 10<s> H2O
```

A simple temperature ramp can be specified directly in the `diffuse` command using the `ramprate` keyword, which sets the change in the temperature over time:

```
diffuse temperature= 900<C> time= 10<min> O2 ramrate= 10<C/min>
```

This example describes a dry oxidation of 10 minutes, starting at 900°C and ending at 1000°C. The same example can be repeated using the `temp_ramp` command as follows:

```
temp_ramp name= MyTempRamp temperature= 900 time= 10 O2 ramrate= 10<C/min>
diffuse temp.ramp= MyTempRamp
```

The first line creates a temperature ramp with given conditions, and the second line specifies a diffusion referring to this temperature ramp.

To describe more complex temperature cycles within one `diffuse` command, multiple instances of the `temp_ramp` command can be used. A temperature ramp can consist of several segments and, for each segment, one `temp_ramp` command is required. In addition, segments can be grouped by using the same name for each segment. For example, a ramp-up, plateau, and ramp-down can be specified as:

```
temp_ramp name= MyCycle temperature= 500<C> time= 5<min> H2O \
    ramrate= 100<C/min>
temp_ramp name= MyCycle temperature= 1000<C> time= 10<min> O2
temp_ramp name= MyCycle temperature= 1000<C> time= 10<min> \
    ramrate= -50<C/min> last
diffuse temp.ramp= MyCycle
```

The `last` option in the third `temp_ramp` command declares the last segment of the temperature ramp.

Sentaurus Process allows for thermal oxidation from O<sub>2</sub> and H<sub>2</sub>O. The `gas_flow` command is used to specify a mixed gas flow by specifying directly either the partial pressures of the gas components or the flow [volume/time]. If the flows are defined, they are converted to partial

pressures by taking ratios. The use of the `gas_flow` command is similar to the `temp_ramp` command; however, multiple gas flows using the same name must not be specified. When a `gas_flow` is specified, it can be referred to from both the `temp_ramp` and `diffuse` commands:

```
gas_flow name= MyGasFlow pH2O= 0.5 pO2= 0.5 pH2= 0.1
```

To invoke the gas flow specification as given above, use:

```
temp_ramp name= MyTempRamp temperature= 1000<C> time= 10<min> \
    gas.flow= MyGasFlow
diffuse temp.ramp= MyTempRamp
```

or:

```
diffuse temperature= 1000<C> time= 10<min> gas.flow= MyGasFlow
```

Sentaurus Process also allows you to select various diffusion models for point defects and dopants (see [Transport Models on page 175](#)). Diffusion model setting and parameter setting are performed with the `pdbSet` command. The basic settings are:

```
pdbSet <material> Dopant DiffModel <model>
```

where `<model>` can be any of Constant, Fermi, Pair, React, ChargedFermi, ChargedPair, or ChargedReact.

Epitaxy can be simulated if either the `Epi` (also known as `epi`) or `LTE` ambient is specified in either the `temp_ramp` or `diffuse` command. If `Epi` is specified, `Silicon` will grow on `Silicon` and `PolySilicon` will grow on `PolySilicon`. If the `LTE` ambient is specified, `Silicon` will again grow on `Silicon`, but `PolySilicon` will grow on `Oxide`, `Nitride`, and `PolySilicon`.

```
pdbSet Silicon Dopant DiffModel Pair
diffuse temperature= 800<C> time= 60<min> Epi thick= 0.01 \
    epi.doping= {Germanium=8e21}
```

This example sets the dopant diffusion model for all dopants in silicon to the `Pair` model and grows a 0.01  $\mu\text{m}$  thick epi layer with a Germanium concentration of  $8 \times 10^{21}$ .

It is also possible to set the initial diffusion time-step and the minimum annealing temperature with the `diffuse` command.

```
diffuse temp.ramp= MyCycle minT= 600<C> init= 0.01<s>
```

This example uses the `temp_ramp` created in the earlier example. The initial time step is set to 0.01 s and the minimum annealing temperature is set to 600°C. The diffusion and reaction equations will be switched off below 600°C but the mechanics will be solved.

## 4: Diffusion

### Basic Diffusion

To set the minimum annealing temperature and initial time-step globally for all diffusion commands, use the following commands:

```
pdbSet Diffuse minT <n>
pdbSet Diffuse InitTimeStep <n>
```

It is also possible to set the minimum and maximum temperature limits for the annealing process using the following commands:

```
pdbSet Diffuse minAnnealT <n>
pdbSet Diffuse maxAnnealT <n>
```

If the annealing temperature goes above or below these limits, Sentaurus Process will quit with an error message.

See [Parameter Database Browser: Viewing the Defaults on page 31](#) for other parameters related to `Diffuse`.

---

## Obtaining Active and Total Dopant Concentrations

By default, active and total dopant concentrations are updated only during diffusion steps. For example, after an implantation, the active concentrations (`BoronActiveConcentration`, `ArsenicActiveConcentration`, and so on) and the total concentrations (`BoronConcentration`, `ArsenicConcentration`, and so on) are not modified, which makes them out of date.

Similarly for other commands that can change the dopant concentrations, the active and total concentrations are not updated. These commands include, but are not limited to, `select`, `load`, `init`, and `profile`.

After one of these commands is issued, the active and total dopant concentrations might not be current. To update the active and total dopant concentrations, use the `diffuse time=0 ...` command.

**NOTE** To update the active and total concentrations of the dopants without dopant redistribution, the `diffuse` command with zero time can be used. For example, to calculate the active dopant concentration at 850°C for the chosen diffusion model, use:

```
diffuse time= 0.0 temperature= 850
```

**NOTE** Since the `diffuse` command performs the recrystallization and the initialization of clusters even with zero time, it must not be added between consecutive implantation steps.

---

## Transport Models

Sentaurus Process has several basic transport models with varying levels of complexity for computing flux,  $\mathbf{J}$ . This diversity of models is needed to balance accuracy with simulation times, which vary widely depending on the model selection:

- The React (see [React Diffusion Model on page 183](#)) and ChargedReact (see [ChargedReact Diffusion Model on page 176](#)) diffusion models, also known as five-stream diffusion models, are the most advanced dopant diffusion models in Sentaurus Process. They solve up to three separate equations per dopant – a substitutional dopant – and up to two dopant–defect pairs and two defect equations. The ChargedReact model is the most accurate model available in Sentaurus Process, but because of the large number of equations required, it also is the most computationally expensive. The React model, which is an uncharged version of the ChargedReact model, is provided for backward compatibility.
- The Pair (see [Pair Diffusion Model on page 187](#)) and ChargedPair (see [ChargedPair Diffusion Model on page 185](#)) diffusion models, also known as three-stream diffusion models, assume that dopant–defect pairs are in local equilibrium but still solve for separate point-defect equations. These models solve one equation per dopant and two defect equations. The ChargedPair diffusion model allows the pairing coefficients to vary with charge state. These models are the most commonly used for advanced CMOS processes as they represent a balance between accuracy and computational expense. For extremely fast ramp rates or for customized initial conditions, the ChargedReact model or React model is a better choice. The Pair model, which is an uncharged version of the ChargedPair model, is provided for backward compatibility.
- The Fermi and ChargedFermi diffusion models are trimmed versions of the Pair and the ChargedPair diffusion models. In certain use cases (for details, see [ChargedFermi Diffusion Model on page 188](#) and [Fermi Diffusion Model on page 190](#)), both models assume that point defects as well as dopant–defect pairs are in equilibrium. The ChargedFermi diffusion model allows the diffusivity of each charge state to be set separately. An uncharged version of the model is provided for backward compatibility. These models can be used for long-term high-temperature anneals where the transient effect of annealing implantation damage is minimal.
- The Constant diffusion model (see [Constant Diffusion Model on page 191](#)), unlike all other transport models, assumes a constant diffusivity and no electric-field effect, and is used mainly for dopant diffusion in oxide.

The selection of transport model is specified as follows:

```
pdbSet <material> Dopant DiffModel <model>
```

where <model> must be one of the valid diffusion model names: Constant, Fermi, Pair, React, ChargedFermi, ChargedPair, or ChargedReact.

## 4: Diffusion

### Basic Diffusion

It is also possible to select a different diffusion model for each dopant in the same material. In this case, use the command:

```
pdbSet <material> <dopant> DiffModel <model>
```

where <dopant> is a valid dopant name (for example, Boron).

The ChargedFermi, ChargedPair, and ChargedReact diffusion models take into account each charged point defect individually. Otherwise, they are very similar to the Fermi and Pair diffusion models.

**NOTE** Even though you can select any diffusion model individually for each dopant, it is not recommended to mix the ChargedFermi, ChargedPair, or ChargedReact models with the uncharged versions.

In [Table 11](#), <material> is a valid material name, <defect> is either Int or Vac, and <dopant> is a valid dopant name.

Table 11 Summary of dopant diffusion models and parameters

Parameter Database command	Type	Diffusion model						
		ChargedReact	React	ChargedPair	Pair	ChargedFermi	Fermi	Constant
pdbSet <material> <defect> ChargeStates	Charging Coeff.	X	X	X	X	X		
pdbSet <material> <defect> ChargeStatesScale	Charging Coeff.	X	X	X	X	X		
pdbSet <material> <defect> Cstar	Concentration	X	X	X	X	X	X	X
pdbSet <material> <defect> D	Diffusivity	X	X	X	X	X		
pdbSet <material> <defect> KbulkChargeStates	Charging Coeff.	X	X	X	X	X		
pdbSet <material> <dopant> <defect> Binding	Pairing Coeff.		X		X			
pdbSet <material> <dopant> <defect> ChargePair	Pairing Coeff.	X		X				
pdbSet <material> <dopant> <defect> D	Diffusivity	X	X	X	X			
pdbSet <material> <dopant> <defect> Dstar	Diffusivity					X	X	
pdbSet <material> <dopant> <defect> kfFTM	Rate	X						
pdbSet <material> <dopant> <defect> kfKickOut	Rate	X						
pdbSet <material> <dopant> Dstar	Diffusivity							X

---

## Recombination and Reaction Models

Many reactions and recombination models are available. Different diffusing species such as dopants, defects, and impurities will all have different recombination and reaction terms. These terms come from the following models:

- Dopant clusters—solid solubility, transient, and dopant–defect cluster models (see [Dopant Activation and Clustering on page 276](#)).
- Defect clusters—Equilibrium, {311}, Loop, LoopEvolution, 1Moment, 2Moment, Full, and FRENDETECH models (see [Defect Clusters on page 306](#)).
- Impurity species:
  - Carbon model, nitrogen model (see [NeutralReact Diffusion Model on page 192](#)).
  - Fluorine model (see [Dopant Active Model: FVCluster on page 291](#)).

---

## Boundary Conditions

Sentaurus Process can simulate various boundary conditions for dopants and defects. You can select from the following boundary conditions:

- HomNeumann can be applied to any boundary (see [HomNeumann on page 344](#)).
- Natural is for point defects (see [Natural on page 344](#)).
- Segregation is for dopants (see [Segregation on page 348](#)).
- Dirichlet is for dopants and defects (see [Dirichlet on page 351](#)).
- ThreePhaseSegregation is for dopants (see [ThreePhaseSegregation on page 352](#)).
- GrainBoundarySegregation is for dopants in polycrystalline materials (see [Boundary Conditions on page 239](#)).
- GrainGrainBoundarySegregation is for dopants in polycrystalline materials (see [Boundary Conditions on page 239](#)).
- Trap is for dopants such as fluorine and nitrogen in trap-dependent oxidation.
- TrapGen is for dopants such as nitrogen in N<sub>2</sub>O oxidation.
- Continuous is for dopants used only during epi growth (see [Continuous on page 358](#)).

The Natural and Dirichlet boundary conditions consider interstitial injection during oxidation for oxidation-enhanced diffusion (OED) of dopants.

---

## Other Materials and Effects

In addition to generic transport and recombination and reaction models, other effects can be simulated:

- Polysilicon model (see [Diffusion in Polysilicon on page 224](#)).
  - SiGe diffusion model (see [Dopant Diffusion in Silicon Germanium on page 241](#)).
  - Epitaxy (see [Epitaxy on page 267](#)).
- 

## General Formulation

The general expression for the particle current of a diffusing species  $A$  of charge  $c$  is given by:

$$\mathbf{J}_{A^c} = -d_{A^c} \left( \frac{n}{n_i} \right)^{-c} \nabla \left( A^c \left( \frac{n}{n_i} \right)^c \right) \quad (109)$$

where  $A^c$  is the concentration,  $d_{A^c}$  is the diffusivity,  $n$  is the electron concentration, and  $n_i$  is the intrinsic electron concentration.

The continuity equation for species  $A$  of charge  $c$  is given by:

$$\frac{\partial A^c}{\partial t} = -\nabla \bullet \mathbf{J}_{A^c} + R_{A^c}^{trans} - R_{A^c}^{clus} \quad (110)$$

where the recombination/reaction term is split into two parts:  $R_{A^c}^{trans}$  is a possible contribution coming from the transport model selection (see [Transport Models on page 175](#)) and  $R_{A^c}^{clus}$  can contain terms from other reactions, which are most often clustering reactions but could include any type of reaction. Reactions that transform species  $A^c$  into another species will introduce positive terms into the expression for  $R_{A^c}^{clus}$ . Total dopant concentration of dopant  $A$  will be equal to the sum of all dopants, dopant–defect pairs, and any related clusters (for example,  $A_{Total}^c = A^c + A_{pair}^c + A_{clus}^c$ ).

For the models that do not consider different charge states, computation of the electron concentration by default is given by the charge neutrality condition  $-n + p + \Delta N = 0$ , where  $\Delta N$  is given by the active dopant concentrations (for example,  $\Delta N = N_d - N_a$  where  $N_d$  is the active donor concentration and  $N_a$  is the active acceptor concentration). For the charged models, the charge states of the defects or defect pairs are considered individually.

It is expected that the charge reactions are in equilibrium, so that the ratio in the various charge states is set by the Fermi level:

$$A^{c+r} = k_{A^c} A^r \left( \frac{n}{n_i} \right)^{-(c)} \quad (111)$$

where  $r$  is a reference charge state, which is chosen as 0 for interstitials and vacancies, and is chosen as the dopant charge for dopant–defect pairs. The  $k_{A^c}$  are parameters that are set by default to an Arrhenius expression. In addition, for the charged models, it is necessary to solve a coupled equation for the electron concentration. The default equation is the same as for the uncharged case, that is, the charge neutrality equation  $-n + p + \Delta N = 0$  but, in this case,  $\Delta N$  is a function of  $n$  because it contains contributions from charged defects or charged defect pairs as well as dopants. It is also possible for both the charged and uncharged models to solve the Poisson equation (see [Electron Concentration on page 260](#)).

## Transport Models

Transport models compute the particle flux of dopants and are the core diffusion models solved by Sentaurus Process. In addition to particle flux, pairing reactions can be computed depending on the transport model selection. Transport models are usually used with one or more clustering or activation models available. The reaction or clustering models will not modify the dopant flux, but will compute terms to be added to  $R_{clus}^c$  from [Eq. 110](#). The models are described in detail here.

The selection of the transport model is made with the command:

```
pdbSet <material> <dopant> DiffModel <model>
```

where:

- <material> is the material name.
- <dopant> can be either "Dopant" to apply to all dopants or a named dopant such as boron, arsenic, phosphorus, antimony, and indium.
- <model> is one of the models: ChargedReact, React, ChargedPair, Pair, ChargedFermi, Fermi, or Constant.

Table 12 Solution names

Symbol	Boron	Arsenic	Phosphorus	Antimony	Indium
$C_A$	Boron	Arsenic	Phosphorus	Antimony	Indium
$C_{AI}$	BoronInt	ArsenicInt	PhosphorusInt	AntimonyInt	IndiumInt

## 4: Diffusion

### Transport Models

Table 12 Solution names

Symbol	Boron	Arsenic	Phosphorus	Antimony	Indium
$C_{AV}$	BoronVac	ArsenicVac	PhosphorusVac	AntimonyVac	IndiumVac
$C_A^+$	BAActive	AsActive	PAActive	SbActive	InActive

Table 13 Point-defect names

Symbol	Interstitial	Vacancy
$C_X$	Int	Vac
$C_X^*$	EqInt	EqVac
$C_{X^0}^*$	IntNeutralStar	VacNeutralStar
$C_{X^0}$	IntNeutral	VacNeutral

The transport for point defects is computed when `Compute.Point.Defect` is set to 1:

```
pdbSet <material> Compute.Point.Defect <0 | 1>
```

## ChargedReact Diffusion Model

The ChargedReact diffusion model is the most general transport model in Sentaurus Process. The model has an immobile substitutional dopant and up to two mobile charged dopant–defect pair species. Mobile charged point defects are also included in the model.

The following reactions are considered:



The differential equations that are solved in this model are:

$$\frac{\partial C_A}{\partial t} = -R_{AI} - R_{AV} + R_{AI,V} + R_{AV,I} - R_A^{clus} \quad (117)$$

$$\frac{\partial C_{AI}}{\partial t} = -\nabla \bullet \mathbf{J}_{AI} + R_{AI} - R_{AI,V} - R_{AI}^{clus} \quad (118)$$

$$\frac{\partial C_{AV}}{\partial t} = -\nabla \bullet \mathbf{J}_{AV} + R_{AV} - R_{AV,I} - R_{AV}^{clus} \quad (119)$$

$$\frac{\partial C_I}{\partial t} = -\nabla \bullet \mathbf{J}_I - R_{IV} - R_{AI} - R_{AV,I} - R_I^{clus} \quad (120)$$

$$\frac{\partial C_V}{\partial t} = -\nabla \bullet \mathbf{J}_V - R_{IV} - R_{AV} - R_{AI,V} - R_V^{clus} \quad (121)$$

where  $C_A$  is the concentration of substitutional (and assumed to be immobile) dopants,  $C_X$  is the concentration of ‘free’ defects of type  $X$  (either interstitials or vacancies), in other words, those defects not in clusters or pairs. The reaction rates of the different species ( $R$ ) are defined later in this section.

Next, the flux of the mobile defect pair is considered. Working with [Eq. 109, p. 174](#) for the charged pairs, the equation will be written in terms of the total concentration of pairs.

In the ChargedReact model, it is assumed that the dopant–defect pairing reaction is *not* in equilibrium but is solved using a separate PDE. The flux of the pairs is computed from [Eq. 109, p. 174](#):

$$\begin{aligned} \mathbf{J}_{AX} &= -\sum_c \mathbf{J}_{AX^c} \\ &= -\sum_c D_{AX^c} \left( \frac{n}{n_i} \right)^{-c-z} \nabla \left( \frac{C_{AX}}{C_{X^0}^* \sum_q k_{AX^q} k_{X^q} \left( \frac{n}{n_i} \right)^{-q}} \left( \frac{n}{n_i} \right)^z \right) \end{aligned} \quad (122)$$

where  $D_{AX^c}$  is an effective diffusivity of dopant point-defect pairs at charge state  $c$  and is related to the self diffusivity  $d_{AX^c}$  by:

$$\begin{aligned} D_{AX^c} &= C_{X^0}^* k_{AX^c} k_{X^c} d_{AX^c} \\ &= D_{AX^c}^0 \exp \left( \frac{-D_{AX^c}^E}{k_B T} \right) \end{aligned} \quad (123)$$

The following relation defines the pairing coefficients for dopant–defect pairs when pairs  $C_{AX}$  are in equilibrium with substitutional dopants  $C_A$  and point defects  $C_X$ :

$$C_{AX} \equiv C_A^+ C_{X^0} \sum_c k_{AX^c} k_{X^c} \left( \frac{n}{n_i} \right)^{-c} \quad (124)$$

where:

- $X$  is either an interstitial or a vacancy.
- $c$  is the charge state of the point defect.
- $C_A^+$  is the active portion of  $C_A$ .
- $C_{X^0}$  is the concentration of the neutral point defect  $X$ .
- The ionization equilibrium constant  $k_{X^c}$  is given by [Eq. 126, p. 179](#) and [Eq. 127, p. 179](#).

The concentration of pairs is expressed as the sum of pairs in all possible charge states in [Eq. 124](#). When pairs are not in local equilibrium with substitutional dopants and point defects, [Eq. 124](#) is not valid, but it still governs the relative fraction of pairs in each possible charge state of pairs. This reflects the assumption that charge change reactions are very fast, compared to any other reactions, such as diffusion. The pairing coefficients for the dopant–defect pairs with different charge states,  $k_{AX^c}$ , can be modified with the command:

```
pdbSet <material> <dopant> <defect> ChargePair <c> <n>
```

where:

- $<\text{material}>$  is a material name (see [Specifying Materials on page 18](#)).
- $<\text{dopant}>$  is one of the existing Sentaurus Process dopants.
- $<\text{defect}>$  is either Interstitial or Vacancy.
- $<\text{c}>$  is the charge state.
- $<\text{n}>$  is a Tcl expression that returns a number. It can be simply a number.

$C_{X^0}^*$  is the equilibrium concentration of the neutral defects and is related to the total equilibrium intrinsic concentration of defect  $X$  by:

$$C_{X^0}^* = \frac{C_{X(\text{intrinsic})}^*}{\sum_c k_{X^c}} \quad (125)$$

The quantities  $C_{I(\text{intrinsic})}^*$  and  $C_{V(\text{intrinsic})}^*$ , which by default follow an Arrhenius law, can be changed by using the command:

```
pdbSet <material> <defect> Cstar {<n>}
```

To set  $D_{AX^c}$ , use:

```
pdbSet <material> <dopant> <defect> D <c> {<n>}
```

A set of equilibrium-charging constants,  $k_{X^c}$ , for defect  $X$  is defined:

$$C_{X^c} = k_{X^c} C_{X^0} \left( \frac{n}{n_i} \right)^{-c} \quad (126)$$

where  $X$  is either I or V, and  $k_{X^c}$  is the charging coefficient for the defect  $X$  and is given by:

$$k_{X^c} = k_{X^c}^0 \exp\left(\frac{-k_{X^c}^E}{k_B T}\right) \quad (127)$$

To set  $k_{X^c}$ , use:

```
pdbSet <material> <defect> ChargeStates <c> {<n>}
```

**NOTE** The neutral charge state must always be 1.0.

Similar to the pairs, the defect fluxes are computed from [Eq. 109, p. 174](#):

$$\begin{aligned} J_X &= - \sum_c J_{X^c} \\ &= - \frac{\sum_c k_{X^c} D_{X^c} \left( \frac{n}{n_i} \right)^{-c} C_X^*}{\sum_q k_{X^q} \left( \frac{n}{n_i} \right)^{-q}} \nabla \left( \frac{C_X}{C_X^*} \right) \end{aligned} \quad (128)$$

where  $C_X$  is the total concentration of defects that is the sum of the concentrations of defect  $X$  at every charge state and  $D_{X^c}$  is the diffusivity of the defect  $X$  of charge state  $c$  and is given by:

$$\begin{aligned} D_{X^c} &= d_{X^c} \\ &= D_{X^c}^0 \exp\left(\frac{-D_{X^c}^E}{k_B T}\right) \end{aligned} \quad (129)$$

To set  $D_{X^c}$ , use:

```
pdbSet <material> <defect> D <c> { [Arrhenius <prefactor> <energy>] }
```

## 4: Diffusion

### Transport Models

Now, the reaction rates can be written by considering Eq. 112, p. 176 to Eq. 116, p. 176 and the general formula for the rate of all combinations of charge states:

$$A^a + B^b \leftrightarrow AB^c + (c - a - b)e$$

$$R_{A^a, B^b, c} = k_{A^a, B^b, c}^f \left( C_{A^a} C_{B^b} - k_{A^a, B^b, c}^r C_{AB^c} \left( \frac{n}{n_i} \right)^{(c-a-b)} \right) \quad (130)$$

Therefore, summing all possible charge states gives:

$$R_{AX} \equiv -\bar{K}_{AX}^f \left( C_A C_X - \frac{C_{AX}}{\bar{K}_{AX}^r} \right) \quad (131)$$

$$R_{AI, V} \equiv \bar{K}_{AI, V}^f (C_{AI} C_V - \bar{K}_{AX}^r C_I^* C_V^* C_A) \quad (132)$$

$$R_{AV, I} \equiv \bar{K}_{AV, I}^f (C_{AV} C_I - \bar{K}_{AX}^r C_I^* C_V^* C_A) \quad (133)$$

where:

$$\bar{K}_{AX}^f \equiv \frac{\sum_i K_{f_X KO i} k_{X^i} \left( \frac{n}{n_i} \right)^{-i}}{\sum_c k_{X^c} \left( \frac{n}{n_i} \right)^{-c}} \quad (134)$$

$$\bar{K}_{AX}^r \equiv \frac{\sum_i k_{AX^i} k_{X^i} \left( \frac{n}{n_i} \right)^{-i}}{\sum_c k_{X^c} \left( \frac{n}{n_i} \right)^{-c}} \quad (135)$$

$$\bar{K}_{AI, V}^f \equiv \frac{\sum_i \sum_j K_{f_{AI^i, V^j} FT} k_{AI^i} k_{V^j} \left( \frac{n}{n_i} \right)^{-(i+j)}}{\sum_c k_{Af^c} \left( \frac{n}{n_i} \right)^{-c} \sum_z k_{V^z} \left( \frac{n}{n_i} \right)^{-z}} \quad (136)$$

$$\bar{K}_{AV, I}^f \equiv \frac{\sum_i \sum_j K_{f_{AV^i, I^j} FT} k_{AV^i} k_{I^j} \left( \frac{n}{n_i} \right)^{-(i+j)}}{\sum_c k_{AV^c} \left( \frac{n}{n_i} \right)^{-c} \sum_z k_{I^z} \left( \frac{n}{n_i} \right)^{-z}} \quad (137)$$

where  $\bar{K}_{AX}^f$  is the forward reaction rate for the kick-out mechanism, and  $X$  is either interstitial or vacancy,  $\bar{K}_{AI, V}$  and  $\bar{K}_{AV, I}$  are forward reaction rates for the Frank-Turnbull mechanism and  $K_{AX}^r$  is the equilibrium constant.

The forward ( $K_{f_XKOi,j}$ ) kick-out reaction rates can be set by using the following commands:

```
pdbSet <material> <dopant> <defect> kfKickOut <c> {<n>}
```

where  $c$  is the charge state. By default, `kfKickOut` values for each charge state are given as:

$$K_{f_XKOi} \equiv \frac{D_{AX} \sum k_{X'}}{C_{X(\text{intrinsic})}^* k_X \lambda^2} \quad (138)$$

where  $\lambda$  is the hopping length, which can be set using the command:

```
pdbSet <material> <dopant> <defect> lambdaK
```

An alternative simplified formula for the forward reaction rate ( $\bar{K}_{AX}^f$ ) in Eq. 131 can be defined as:

$$\bar{K}_{AX}^f = \frac{\left( \sum_i D_{AX^i} \right) \cdot \text{DiffFactors} \cdot \text{ReactFactor}}{C_X^* \cdot \lambda^2} \quad (139)$$

Here, `DiffFactors` represents the product of all related user-defined diffusion factors, such as `<dopant><defect>DiffFactor` and `<dopant>DiffFactor`. If these factors are not defined, either by users or by `AdvancedCalibration`, their value is set to 1.

`ReactFactor` represents `React<dopant><defect>Factor`. If it is not defined, it is assumed to equal 1. This term provides additional flexibility to control the dependency of the pair formation rate on certain process variables. For example, to enhance phosphorus–vacancy pair formation and dissolution in the presence of arsenic in Si, you can use the following definition:

```
term Si name=ReactPhosphorusVacFactor eqn= "(1.0e20+AsTotal)/1.0e20" add store
```

To use this simplified version of the forward reaction rate, a Boolean parameter has been introduced, which can be set using the command:

```
pdbSet <material> <dopant> Kick.Out.Rate.Based.On.Lambda 1
```

The default value of `Kick.Out.Rate.Based.On.Lambda` is false (0) to maintain backward compatibility.

When `Kick.Out.Rate.Based.On.Lambda` is set to 1, you can define an additional term factor named `<dopant><defect>IonPairFactor`, which, if defined, is multiplied by the corresponding forward reaction term of the pair formation (proportional to  $C_A C_X$ ) in the definition of the overall reaction rate  $R_{AX}$  in Eq. 131.

The simplified implementation of  $\bar{K}_{AX}^f$  in Eq. 139 has advantages compared to Eq. 134 and Eq. 138:

- In Eq. 139, the effective hopping length of dopant-defect pairs (that is, the average distance between pair formation and pair dissociation) is exactly equal to  $\lambda / (\text{sqrt(ReactFactor)})$ . Therefore,  $\lambda$  has a clear physical meaning. It defines the hopping length and, therefore, the steepness of the diffusion tails for thermal anneals with very small thermal budgets. In contrast, when using Eq. 134 and Eq. 138, the hopping length can differ from  $\lambda$ , in particular, when diffusion enhancement factors are defined, and also for dopant-defect pair diffusion in strained Si and SiGe.
- It allows additional flexibility using the `React<dopant><defect>Factor` term.
- It makes the expression for  $\bar{K}_{AX}^f$  shorter, allowing for a small speedup.

Similarly, the forward ( $\bar{K}_{AI,V}^f$ ,  $\bar{K}_{AV,I}^f$ ) Frank-Turnbull reaction rates can be defined using the commands:

```
pdbSet <material> <dopant> <defect> kfFTM <i,j> {<n>}
```

**NOTE** The indices of the forward recombination rates have the form of  $i, j$ . Both  $i$  and  $j$  are integers and are separated by a comma; no space is allowed between the indices.

The  $I-V$  recombination reaction is given as:

$$R_{IV} = \bar{K}_{IV}(C_I C_V - C_I^* C_V^*) \quad (140)$$

where:

$$\bar{K}_{IV} = \frac{C_{I(intrinsic)}^* C_{V(intrinsic)}^*}{C_I^* C_V^* \sum_z k_I \sum_z k_{V^z}} \sum_i \sum_j K_{I^i V^j} k_I k_{V^j} \left(\frac{n}{n_i}\right)^{-(i+j)} \quad (141)$$

The superscript ‘\*’ refers to the equilibrium concentration, and the subscripts  $I$  and  $V$  are for the interstitials and vacancies, respectively. The subscripts  $z, i, j$  are the charge states of the defects.  $K_{I^i V^j}$  is the bulk recombination rate for interstitials and vacancies at the charge stated  $i$  and  $j$ , respectively. The bulk recombination rate  $K_{I^i V^j}$  for each charged point defect can be set using the command:

```
pdbSet <mater> <defect> KbulkChargeStates <i,j> {<n>}
```

The recombination rate is multiplied by the terms `IntBulkRecombinationFactor` and `VacBulkRecombinationFactor`, which equal 1.0 if these terms are not defined. In the Advanced Calibration file, these terms are defined and include common factors applied to all pairs  $<i, j>$  of charge state indices.

The equilibrium concentration of the unpaired point defect can be calculated by:

$$C_X^* = C_{X(intrinsic)}^* \frac{\sum_c k_{X^c} \left(\frac{n}{n_i}\right)^{-c}}{\sum_c k_{X^c}^s} \quad (142)$$

where  $k_{X^c}^s$  is the scaled charging coefficient for the defect  $X$  and can be set by using:

```
pdbSet <material> <defect> ChargeStatesScale <c> {<n>}
```

$k_{X^c}^s$  is set to  $k_{X^c}$  as a default.

**NOTE** The indices for the parameter KbulkChargeStates have the form of  $i, j$ . Both  $i$  and  $j$  are integers and are separated by a comma; no space is allowed between the indices.

## React Diffusion Model

The React model is similar to the ChargedReact model, except that the reaction rates are not charge state-dependent and the electron concentration is computed directly from the net doping concentration. In addition, the Frank–Turnbull mechanism is not considered.

The reactions considered are:



where  $A$  is the dopant,  $I$  is the interstitial, and  $V$  is the vacancy.

The following set of differential equations represents the model:

$$\frac{\partial C_A}{\partial t} = -R_{AI} - R_{AV} - R_A^{clus} \quad (145)$$

$$\frac{\partial C_{AX}}{\partial t} = -\nabla \bullet J_{AX} + R_{AX} - R_{AX}^{clus} \quad (146)$$

$$\frac{\partial C_X}{\partial t} = -\nabla \bullet J_X - R_{IV} - R_{AX} - R_X^{clus} \quad (147)$$

where  $C_A$  is the concentration of substitutional (and assumed to be immobile) dopant and  $C_X$  is the concentration of ‘free’ defects of type  $X$  (either interstitials or vacancies), that is, those defects not in clusters or pairs.

Next, the flux of the mobile–defect pair is considered. In this model, the reaction rates are assumed to be independent of the charge state, so the pair charging constants are only needed for the flux of the pairs and are absorbed into the diffusivity of the pairs in this way:

$$J_{AX} = \frac{-\sum_c \left( D_{AX^c} \left( \frac{n}{n_i} \right)^{c-z} \right)}{B_{AX}} \nabla \frac{C_{AX} \left( \frac{n}{n_i} \right)^z}{C_X^*} \quad (148)$$

where  $z$  is the charge state of dopant  $A$ ,  $X$  is either interstitial or vacancy, and  $D_{AX^c}$  is the effective diffusivity of dopant point-defect pair at charge state  $c$  and is related to the bare diffusivity,  $d_{AX^c}$  by:

$$\begin{aligned} D_{AX^c} &= C_{X^0}^* B_{AX} k_{X^c} d_{AX^c} \\ &= D_{AX^c}^0 \exp\left(\frac{-D_{AX^c}^E}{k_B T}\right) \end{aligned} \quad (149)$$

where  $k_{X^c}$  is a set of equilibrium charging constants for defect  $X$  defined by [Eq. 126, p. 179](#) and [Eq. 127, p. 179](#), and  $C_{X^0}^*$  is the equilibrium concentration of the neutral defects defined by [Eq. 125, p. 178](#).

To set  $D_{AX^c}$ , use:

```
pdbSet <material> <dopant> <defect> D <c> {<n>}
```

where:

- <material> is a material name (see [Specifying Materials on page 18](#)).
- <dopant> is one of the existing Sentaurus Process dopants.
- <defect> is either Interstitial or Vacancy.
- <c> is the charge state.
- <n> is a Tcl expression that returns a number; it can be simply a number.

The commonly used Tcl procedure Arrhenius is used to set parameters, and it takes a prefactor and an energy as arguments, and returns  $\text{prefactor} \cdot \exp\left(\frac{-\text{energy}}{k_B T}\right)$ .

You can modify the entire array with the command (for example, arsenic–vacancy pairs):

```
 pdbSet Si Arsenic Vac D {
    0 {[Arrhenius 0.0 3.45]}
    -1 {[Arrhenius 12.8 4.05]}
}
```

The defect flux  $J_X$  is the same as the ChargedReact model and is given by [Eq. 128, p. 179](#). The reaction can be written as:

$$R_{AX} \equiv K_{AXr} \left( C_A^+ C_X - \frac{C_{AX}}{B_{AX}} \right) \quad (150)$$

where  $X$  is either interstitial or vacancy,  $B_{AX}$  is the binding coefficient of defect  $X$  and dopant  $A$ ,  $K_{AXr}$  is the rate constant for the chemical reaction, and  $C_A^+$  is the active portion of  $C_A$ .

The binding term between the defect and dopant also follows the Arrhenius law:

$$B_{AX} = B_{AX0} \exp\left(\frac{-B_{AXE}}{kT}\right) \quad (151)$$

The term can be changed with the command:

```
 pdbSet <material> <dopant> <defect> Binding <n>
```

The chemical reaction term is expressed with:

$$K_r = K_{r0} \exp\left(\frac{-K_{rE}}{kT}\right) \quad (152)$$

and can be modified by using the command:

```
 pdbSet <material> <dopant> <defect> Krate <n>
```

The defect recombination rate  $R_{IV}$  is the same as in the ChargedReact model and is given by [Eq. 140, p. 182](#).

## ChargedPair Diffusion Model

The ChargedPair diffusion model assumes that the dopant–defect pairs are in local equilibrium with the dopant and defect concentration. Point defects themselves are not assumed to be in equilibrium. The kick-out mechanism that describes the dopant–defect pairing is given by:



## 4: Diffusion

### Transport Models



and is assumed to be in equilibrium. In these two equations,  $A$  is the dopant,  $I$  is the interstitial,  $V$  is the vacancy, and  $c$  is the charge state.

The differential equations solved with this model are:

$$\frac{\partial C_A}{\partial t} = -\nabla \bullet \mathbf{J}_A - R_A^{clus} \quad (155)$$

$$\frac{\partial}{\partial t}(C_{X^{total}}) = -\nabla \bullet \mathbf{J}_X - \nabla \bullet \mathbf{J}_A - R_{IV} - R_X^{clus} \quad (156)$$

where  $C_{X^{total}} \equiv C_X + C_{AX}$  is the total interstitial concentration including dopant–defect  $X$  pairs but excluding clusters,  $\mathbf{J}_A$  is the sum of AI and AV pair fluxes,  $\mathbf{J}_X$  is the defect flux, and  $C_A$  is the total dopant concentration excluding clusters.

To write an expression for the pair fluxes, it is necessary to first define the equilibrium condition as in [Eq. 124, p. 178](#).

The flux for the impurity is given by:

$$\mathbf{J}_A = -\sum_{c,X} D_{AX^c} \left(\frac{n}{n_i}\right)^{-c-z} \nabla \left( C_A^+ \frac{C_{X^0}}{C_{X^0}^*} \left(\frac{n}{n_i}\right)^z \right) \quad (157)$$

where  $D_{AX^c}$  is the effective diffusivity of dopant point-defect pair at charge state  $c$ ,  $z$  is the charge state of dopant  $A$ ,  $C_A^+$  is the active portion of  $C_A$ ,  $C_{X^0}$  is the concentration of the neutral point defect  $X$ , and  $C_{X^0}^*$  is the equilibrium concentration of the same defect and is given by [Eq. 125, p. 178](#).

The effective diffusivity is related to the bare dopant–defect diffusivity,  $d_{AX^c}$ , by:

$$\begin{aligned} D_{AX^c} &= C_{X^0}^* k_{X^c} k_{AX^c} d_{AX^c} \\ &= D_{AX^c}^0 \exp\left(\frac{-D_{AX^c}^E}{k_B T}\right) \end{aligned} \quad (158)$$

You can set  $D_{AX^c}$  using:

```
pdbSet <material> <dopant> <defect> D <c> <n>
```

**NOTE** Diffusion coefficients  $D$  for the ChargedPair model and  $Dstar$  for the ChargedFermi model include the interstitial efficiency factors.

Both the flux for the defects ( $\mathbf{J}_X$ ) and the defect recombination rate ( $R_{IV}$ ) are the same as the ChargedReact model and are given by [Eq. 128, p. 179](#) and [Eq. 140, p. 182](#), respectively.

## Pair Diffusion Model

The Pair diffusion model is similar to the ChargedPair model except that the reaction rates are not charge state-dependent, and the electron concentration is computed directly from the net doping concentration. In addition, the Frank–Turnbull mechanism is not considered. The kick-out mechanism, which describes the dopant–defect pairing, is given by:



and is assumed to be in equilibrium. In these two equations,  $A$  is the dopant,  $I$  is the interstitial, and  $V$  is the vacancy.

As in the ChargedPair model, the following set of differential equations is solved:

$$\frac{\partial C_A}{\partial t} = -\nabla \bullet \mathbf{J}_A - R_A^{clus} \quad (161)$$

$$\frac{\partial}{\partial t}(C_{X^{total}}) = -\nabla \bullet \mathbf{J}_X - \nabla \bullet \mathbf{J}_A - R_{IV} - R_X^{clus} \quad (162)$$

where  $C_{X^{total}} \equiv C_X + C_{AX}$  is the total interstitial concentration including dopant–defect  $X$  pairs but excluding clusters,  $\mathbf{J}_A$  is the sum of AI and AV pair fluxes,  $\mathbf{J}_X$  is the defect flux, and  $C_A$  is the total dopant concentration excluding clusters.

An equilibrium constant for the pairing reactions is defined and given by:

$$C_{AX} \equiv B_{AX} C_A^+ C_X \quad (163)$$

where  $X$  is either interstitial or vacancy,  $B_{AX}$  is the binding coefficient of defect  $X$  and dopant  $A$ , and  $C_A^+$  is the active portion of  $C_A$ .

The binding term between the defect and dopant also follows the Arrhenius law:

$$B_{AX} = B_{AX0} \exp\left(\frac{-B_{AXE}}{kT}\right) \quad (164)$$

The term can be changed with the command:

```
pdbSet <material> <dopant> <defect> Binding {<n>}
```

The flux for the impurity is given by:

$$\mathbf{J}_A = - \sum_{c, X} D_{AX^c} \left( \frac{n}{n_i} \right)^{-c-z} \nabla \left( C_A^+ \frac{C_X}{C_X^*} \left( \frac{n}{n_i} \right)^z \right) \quad (165)$$

where  $D_{AX^c}$  represents the diffusivity of dopant point-defect pairs at charge state  $c$ ,  $z$  is the charge state of dopant  $A$ ,  $C_A^+$  is the active portion of  $C_A$ , and  $X$  is either interstitial or vacancy. The effective diffusivity is related to the bare dopant–defect diffusivity,  $d_{AX^c}$ , by:

$$\begin{aligned} D_{AX^c} &= C_{X^0}^* k_{X^c} B_{AX} d_{AX^c} \\ &= D_{AX^c}^0 \exp\left(\frac{-D_{AX^c}^E}{k_B T}\right) \end{aligned} \quad (166)$$

where  $C_{X^0}^*$  is the equilibrium concentration of the neutral point defect  $X$  and the ionization equilibrium constant,  $k_{X^c}$ , is defined by [Eq. 126, p. 179](#) and [Eq. 127, p. 179](#).

To modify diffusivity terms, use the command:

```
pdbSet <material> <dopant> <defect> D <charge> {<n>}
```

Both the flux for the defects ( $\mathbf{J}_X$ ) and the defect recombination rate ( $R_{IV}$ ) are the same as the ChargedReact model and are given by [Eq. 128, p. 179](#) and [Eq. 140, p. 182](#), respectively.

## ChargedFermi Diffusion Model

The ChargedFermi diffusion model is similar to the ChargedPair diffusion model. The dependency of diffusivities on the electron and hole concentration is taken into account with the following exceptions:

- No point-defect equations are solved, and point defects are considered to be in equilibrium for inert anneals, if the point-defect clusters are switched off.
- Only the interstitial point-defect equation is solved, and vacancies are considered to be in equilibrium for oxidizing anneals, if the point-defect clusters are switched off.
- Both point-defect equations are solved if the point-defect clusters are switched on.

**NOTE** If the point-defect equations are solved, the transport of point defects by diffusion of dopant–defect pairs is ignored.

The substitutional dopants are immobile and the total dopant flux is due to the dopant–defect pairs. The following set of differential equations is solved along with the potential equation Eq. 369, p. 261:

$$\frac{\partial C_A}{\partial t} = -\nabla \bullet \mathbf{J}_A \quad (167)$$

As in the ChargedPair model, a set of pairing constants ( $k_{AX^c}$ ) that define the pair concentration is defined:

$$C_{AX} \equiv C_A^+ C_{X^0} \sum_c k_{AX^c} k_{X^c} \left( \frac{n}{n_i} \right)^{-c} \quad (168)$$

where:

- $X$  is either interstitial or vacancy.
- $c$  is the charge state of the point defect.
- $z$  is the charge state of dopant  $A$ .
- $C_A^+$  is the active portion of  $C_A$ .

The ionization equilibrium constant  $k_{X^c}$  is given by Eq. 126, p. 179 and Eq. 127, p. 179.

The dopant flux  $\mathbf{J}_A$  is given by:

$$\mathbf{J}_A = - \sum_{c, X} D_{AX^c} \left( \frac{n}{n_i} \right)^{-c-z} \nabla \left( C_A^+ \frac{C_{X^0}}{C_{X^0}^*} \left( \frac{n}{n_i} \right)^z \right) \quad (169)$$

where:

- $D_{AX^c}$  is the effective diffusivity of dopant point–defect pairs at charge state  $c$ .
- $C_{X^0}$  is the concentration of the neutral point defect  $X$ .
- $C_{X^0}^*$  is the equilibrium concentration of the same defect and is given by Eq. 125, p. 178.
- $C_{X^0}$  will be equal to  $C_{X^0}^*$  if the point-defect equations are switched off.
- $D_{AX^c}$  is related to the bare diffusivity  $d_{AX^c}$  by:

$$\begin{aligned} D_{AX^c} &= C_{X^0}^* k_{AX^c} k_{X^c} d_{AX^c} \\ &= D_{AX^c}^0 \exp \left( \frac{-D_{AX^c}^E}{k_B T} \right) \end{aligned} \quad (170)$$

To set  $D_{AX^c}$  use:

```
pdbSet <material> <dopant> <defect> Dstar <c> {<n>}
```

The pairing coefficients for the dopant–defect pairs with different charge states,  $k_{AX^c}$ , can be defined with the command:

```
pdbSet <material> <dopant> <defect> ChargePair <c> {<n>}
```

## Fermi Diffusion Model

The Fermi diffusion model is more complex than the Constant diffusion model. The dependency of diffusivities on the electron and hole concentration is taken into account with the following exceptions:

- No point-defect equations are solved, and point defects are considered to be in equilibrium for inert anneals, if the point-defect clusters are switched off.
- Only the interstitial point-defect equation is solved, and vacancies are considered to be in equilibrium for oxidizing anneals, if the point-defect clusters are switched off.
- Both point-defect equations are solved if the point-defect clusters are switched on.

**NOTE** If the point-defect equations are solved, the transport of point defects by diffusion of dopant–defect pairs is ignored.

As in the ChargedPair model, the following set of differential equations is solved:

$$\frac{\partial C_A}{\partial t} = -\nabla \cdot \mathbf{J}_A \quad (171)$$

where  $\mathbf{J}_A$  is the sum of AI and AV pair fluxes, and  $C_A$  is the total dopant concentration including clusters.

An equilibrium constant for the pairing reactions is defined and given by:

$$C_{AX} \equiv B_{AX} C_A^+ C_X \quad (172)$$

where  $X$  is either interstitial or vacancy,  $B_{AX}$  is the binding coefficient of defect  $X$  and dopant A, and  $C_A^+$  is the active portion of  $C_A$ . The dopant flux is given by:

$$\mathbf{J}_A = -\sum_{X,c} D_{AX^c} \left( \frac{n}{n_i} \right)^{-c-z} \nabla \left( C_A^+ \left( \frac{n}{n_i} \right)^z \right) \quad (173)$$

where:

- $c$  is the charge state of the point defect.
- $z$  is the charge state of dopant A .
- $C_A^+$  is the active portion of  $C_A$  .

- $X$  is either interstitial or vacancy.
- $D_{AX^c}$  is the effective diffusivity of dopant point-defect pairs at charge state  $c$  and is related to the bare diffusivity  $d_{AX^c}$  by:

$$\begin{aligned} D_{AX^c} &= C_{X^0}^* B_{AX} k_{X^c} d_{AX^c} \\ &= D_{AX^c}^0 \exp\left(\frac{-D_{AX^c}^E}{k_B T}\right) \end{aligned} \quad (174)$$

The pairing ratio  $B_{AX}$  only appears in the formula for  $D$  and cannot be modified independently in the Fermi model. You can set  $D_{AX^c}$  using:

```
pdbSet <material> <dopant> <defect> Dstar <c> {<n>}
```

## Constant Diffusion Model

The Constant diffusion model is the simplest diffusion model used in Sentaurus Process and is mainly for dopant diffusion in oxide. It assumes that there is no interaction between dopants and point defects, and that there are no electric-field effects on dopant diffusion. The point-defect equations are also switched off. The impurity diffusion is given by:

$$\frac{\partial C_A}{\partial t} = \nabla \bullet (D_{star} \nabla C_A^+) \quad (175)$$

where  $D_{star}$  is the intrinsic diffusivity of the impurity  $A$ , and  $C_A^+$  is the active portion of  $C_A$ . The diffusivity follows the Arrhenius law:

$$D_{star} = D_{star0} \exp\left(\frac{-D_{starE}}{kT}\right) \quad (176)$$

For example, the following command sets  $D_{star0}$  to  $6.66 \times 10^{-2} \text{ cm}^2/\text{s}$  and  $D_{starE}$  to 3.44 eV:

```
pdbSet Silicon Arsenic Dstar {[Arrhenius 6.66e-2 3.44]}
```

The general format of the command is:

```
pdbSet <material> <dopant> Dstar {<n>}
```

**NOTE** Unlike the ChargedFermi model, Dstar is not defined as an array for the Constant model.

## NeutralReact Diffusion Model

NeutralReact diffusion in silicon is close to the React model (see [React Diffusion Model on page 183](#)) except that there are no charged atoms. The model can be switched on using the command:

```
pdbSet <material> <dopant> DiffModel NeutralReact
```

NeutralReact diffusion in silicon is described by a kick-out mechanism [1]. Other mechanisms such as dissociation and clustering can also be taken into account. In the integration in Sentaurus Process, each of these mechanisms is described by one or more terms:



where  $A$  is the substitutional dopant,  $AI$  is the mobile dopant–interstitial pair,  $I$  is interstitial, and  $V$  is vacancy. The first reaction is the kick-out reaction and the second one is the dissociation reaction. These reaction can be written as:

$$R_{KickOut} \equiv K_{fI}(C_A C_I - B_{AI} C_{AI}) \quad (179)$$

$$R_{Dissociation} \equiv K_{fV}(C_{AI} C_V - C_I^* C_V^* B_{AV} C_A) \quad (180)$$

where:

- $C_A$  is the concentration of substitutional dopant atoms.
- $C_{AI}$  is the concentration of mobile dopant atoms.
- $K_{fI}$  and  $K_{fV}$  are the forward reaction rates.
- $B_{AI}$  and  $B_{AV}$  are the binding coefficients.

To set, use:

```
pdbSet <material> <dopant> Interstitial Kf {<n>}
pdbSet <material> <dopant> Vacancy Kf {<n>}
pdbSet <material> <dopant> Interstitial Bind {<n>}
pdbSet <material> <dopant> Vacancy Bind {<n>}
```

The differential equations that describe the model are:

$$\frac{\partial C_A}{\partial t} = R_{Dissociation} - R_{KickOut} \quad (181)$$

$$\frac{\partial C_{AI}}{\partial t} = \nabla \bullet (D_{AI^0} \nabla C_{AI}) + R_{KickOut} - R_{Dissociation} \quad (182)$$

where  $D_{AI^0}$  is the diffusivity of mobile dopant–interstitial pairs and can be set using the command:

```
pdbSet <material> <dopant> Interstitial D 0 {<n>}
```

## Carbon Diffusion Model

Carbon diffusion is a typical example for the NeutralReact diffusion model. The kick-out reaction rate is defined by:

```
pdbSet Silicon Carbon Interstitial Kf {\ \
  [expr ([pdbGetElement Si Carbon D 0]/([pdbDelayDouble Si Carbon\ \
  MigrationLength]* [pdbDelayDouble Si Carbon\ \
  MigrationLength]* [pdbDelayDouble Si Int Cstar]))]\ \
}
```

It will set  $K_{fl}$  to  $\frac{D_{C^0}}{\lambda^2 C_I^{*}(intrinsic)}$ .

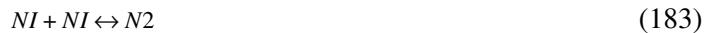
$\lambda$  is the migration length (cm) of carbon atoms and  $D_{C^0}$  is the diffusivity of carbon, and these parameters can be set using the commands:

```
pdbSet <material> Carbon MigrationLength {<n>} \
  pdbSet <material> Carbon D 0 {<n>}
```

For the details of the carbon-clustering model, see [Carbon Cluster on page 290](#).

## Nitrogen Diffusion Model

Nitrogen diffusion is defined according to the Constant diffusion model by default. However, instead of the Constant model, the NeutralReact diffusion model can be used for nitrogen diffusion. If the NeutralReact model is specified for nitrogen diffusion, the nitrogen dimer forms and diffuses. The dimer is formed by the following reaction:



In the above reaction,  $NI$  is the monomer, in other words, nitrogen interstitial  $N_i$ , and  $N2$  denotes the dimer  $(N_i)_2$ , which has the solution name NDimer. The nitrogen monomer and dimer equations are formulated by:

$$\frac{\partial C_N}{\partial t} = R_{Dissociation} - R_{KickOut} - R_{NV} \quad (184)$$

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$$\frac{\partial C_{NI}}{\partial t} = \nabla \bullet (D_{NI}^0 \nabla C_{NI}) + R_{KickOut} - R_{Dissociation} - R_{N2} \quad (185)$$

$$\frac{\partial C_{N2}}{\partial t} = \nabla \bullet (D_{N2} \nabla C_{N2}) + R_{N2} - R_{N2V} \quad (186)$$

$$\frac{\partial C_{N2V}}{\partial t} = R_{N2V} - R_{N2V2} \quad (187)$$

$$\frac{\partial C_{N2V2}}{\partial t} = R_{N2V2} \quad (188)$$

The reaction  $R_{N2}$  for dimer formation is given by:

$$R_{N2} \equiv K_{fN2}(C_{NI}C_{NI} - B_{N2}C_{N2}) \quad (189)$$

where:

- $C_{NI}$  is the concentration of nitrogen monomers.
- $C_{N2}$  is the concentration of nitrogen dimers.
- $K_{fN2}$  is the forward reaction rate.
- $B_{N2}$  is the binding coefficient.

To set, use:

```
pdbSet <material> NDimer Kf {<n>}
pdbSet <material> NDimer Bind {<n>}
```

**NOTE** NDimer is a cluster of nitrogen that can be diffused using the NeutralReact diffusion model and is initialized by nitrogen cluster initialization. For details about nitrogen clusters including NV, N<sub>2</sub>V, and N<sub>2</sub>V<sub>2</sub>, see [Nitrogen Cluster on page 291](#).

## ChargedEquilibrium Diffusion Model

ChargedEquilibrium diffusion in silicon is close to the point-defect diffusion model (see [ChargedReact Diffusion Model on page 176](#)). The model can be switched on using the command:

```
pdbSet <material> <dopant> DiffModel ChargedEquilibrium
```

ChargeEquilibrium diffusion in silicon is described by:

$$\frac{\partial C_A}{\partial t} = -\nabla \bullet J_A \quad (190)$$

$$\begin{aligned} J_A &= -\sum_c J_{A^c} \\ &= -\sum_c k_{A^c} D_{A^c} \left(\frac{n}{n_i}\right)^{-c} \nabla \frac{C_A}{\sum_c k_{A^c} \left(\frac{n}{n_i}\right)^{-c}} \end{aligned} \quad (191)$$

As in the point defect model, a set of equilibrium constants ( $k_{A^c}$ ) that define the charged concentration is defined:

$$C_{A^c} = k_{A^c} C_{A^0} \left(\frac{n}{n_i}\right)^{-c} \quad (192)$$

where  $c$  is the charge state of the dopant. To set  $k_{A^c}$  and  $D_{A^c}$ , use:

```
pdbSet <material> <dopant> ChargeStates <c> {<n>}
pdbSet <material> <dopant> Dstar <c> {<n>}
```

## Copper Diffusion Model

Copper diffusion is a typical use of the ChargedEquilibrium diffusion model. The model is given in [2], and it assumes that copper not only diffuses interstitially, but also sits primarily at interstitial sites. Therefore, substitutional copper can be neglected. Copper contamination and precipitation can be detrimental to device performance. For details about the copper precipitation model, see [Dopant Active Model: FullPrecipitation on page 280](#).

### Copper–Boron Pairing

Copper can pair with boron. This pairing reaction affects copper diffusion and precipitation [2]:



In Sentaurus Process, this reaction is modeled with the following differential equation:

$$\frac{\partial C_{\text{CuB}}}{\partial t} = Kf(C_{\text{Cu}}^+ C_{\text{B}}^- - Kb C_{\text{CuB}}) \quad (194)$$

where:

- $C_{\text{CuB}}$  is the concentration of copper–boron pairs.
- $C_{\text{Cu}}^+$  is the concentration of active copper.

- $C_B^-$  is the concentration of active boron.
- $Kf$  and  $Kb$  are the forward reaction rate and the equilibrium constant, respectively.

You can specify the model parameters with the commands:

```
pdbSet Silicon Copper Boron Kf {<n>}
pdbSet Silicon Copper Boron Kb {<n>}
```

## Mobile Impurities and Ion-Pairing

The ion-pairing model includes the pairing of positively and negatively charged dopant ions [3][4][5]. Ion-pairing reduces the diffusivity of dopants where the concentration of dopants of the opposite type is large. The ion-pairing model assumes that positively charged donors can bind with negatively charged acceptors to form neutral pairs. The ion-pairing model is significant because it allows the dependency of the impurity diffusivity to be modeled in both n-type and p-type materials. In particular, it reduces the effective diffusivity of boron in n-type materials without affecting its diffusivity at high p-type concentrations.

The model reduces the mobile concentration of dopant species by the following factors:

$$f_{pd} = \left(1 - \frac{N_p}{N_d}\right) \text{ for donor species} \quad (195)$$

$$f_{pa} = \left(1 - \frac{N_p}{N_a}\right) \text{ for acceptor species} \quad (196)$$

where:

- $N_d$  and  $N_a$  are the total concentrations of electrically active donors and acceptors, respectively.
- $N_p$  is the concentration of ion pairs.
- $f_{pd}$  and  $f_{pa}$  are the ion-pairing factors for donors and acceptors, respectively.

The concentration of ion pairs  $N_p$  is given by:

$$N_p = \frac{1}{2}((N_d + N_a + \Omega) - \sqrt{(N_d + N_a + \Omega)^2 - 4N_d N_a}) \quad (197)$$

The parameter  $\Omega$  is given by:

$$\Omega = \text{Ion.Pair.Omega} \cdot n_i \quad (198)$$

where `Ion.Pair.Omega` is a parameter for material; the default value for silicon and polysilicon is 6.0 [4].

The ion-pairing model is enabled or disabled for each material by the `Ion.Pair` parameter. By default, it is disabled for all materials.

## Solid Phase Epitaxial Regrowth Model

The solid phase epitaxial regrowth (SPER) model simulates the movement of amorphous and crystalline boundaries due to the recrystallization of the amorphous silicon and the dopant dynamics during such process. The SPER model is switched on by:

```
pdbSet Diffuse SPER 1
```

The boundary movement is described with the specific solution fields, either the distance field by the level-set method or the phase field by the phase-field method. You can select one of the models by:

```
pdbSet Diffuse SPER.Model {LevelSet | PhaseField}      ;# default=LevelSet
```

## Level-Set Method

The level-set method solves the equation for the distance field  $\varphi$ , which is named with `AmorpDistance`:

$$\frac{\partial \varphi}{\partial t} + v |\vec{\nabla} \varphi| = 0 \quad (199)$$

where:

- $v$  is the recrystallization velocity perpendicular to a boundary surface.
- $\varphi$  is positive in an amorphous region, negative in a crystalline region, and zero at an amorphous-crystalline boundary.

The velocity  $v$  is defined by:

$$v = f_v \cdot v_{ori}(V100, V110, V111) \cdot \left( 1 - (1 - s_v) \exp\left(-\frac{d}{L_{vr}}\right) \right) \quad (200)$$

where:

- $f_v$  is the scaling factor.
- $v_{ori}$  is the orientation-dependent velocity.
- $s_v$  is the scaling factor of velocity near surfaces.
- $d$  is the shortest distance from the surface.
- $L_{vr}$  is the characteristic length for velocity reduction near surfaces.

#### 4: Diffusion

##### Solid Phase Epitaxial Regrowth Model

```
pdbSet Silicon SPER V.Factor {<expression>}      ;# f_v (unitless)
pdbSet Silicon SPER V100 {<n>}                  ;# cm/s
pdbSet Silicon SPER V110 {<n>}                  ;# cm/s
pdbSet Silicon SPER V111 {<n>}                  ;# cm/s
pdbSet Silicon SPER VsurfScale {<n>}            ;# s_v (unitless)
pdbSet Silicon SPER VsurfScaleLength {<n>}        ;# L_vr (um)
```

The tensor mesh structure to solve the level-set equation is defined by:

```
pdbSet Grid SPER TensorMeshSpacing {X <n> Y <n> Z <n>} ;# um
```

The level-set algorithm used is the general time-stepping initial-value formulation as described in [MGOALS on page 816](#).

It is assumed that all dopant atoms are mobile in an amorphous region. The diffusion coefficient of the mobile species in the amorphous region is specified by:

```
pdbSet Silicon <dopant> DAmor {<n>} ;# cm2/sec
```

It has been experimentally observed that during regrowth of an amorphous layer, dopants can be swept along by the amorphous–crystalline boundary. The physical mechanism for this sweeping behavior is not well understood. To model this effect, a phenomenological model has been introduced as follows:

$$\frac{\partial X}{\partial t} = \vec{\nabla} \cdot \left( f_D \alpha v_D L_d \left( 1 - (1 - P) \exp\left(-\frac{d}{L_{dr}}\right) \right) \vec{X} \vec{\nabla} \alpha_s \right) \quad (201)$$

where:

- $f_D$  is the user-defined multiplication factor.
- $v_D$  is the local speed of distance variation.
- $L_d$  is the characteristic length of dopant drift.
- $P$  is the drift probability near material interfaces.
- $d$  is the shortest distance from material interfaces.
- $L_{dr}$  is the characteristic length for drift reduction near material interfaces.
- $\alpha$  is the amorphous state calculated by:

$$\alpha = \frac{1}{2} \cdot \text{erfc}\left(-\frac{\Phi}{w_T}\right) \quad (202)$$

where  $w_T$  is the phase transition width.  $\alpha$  is 1.0 and 0.0 in a completely amorphous and crystalline region, respectively.

- $\alpha_s$  is the shifted amorphous state given by:

$$\alpha_s = \frac{1}{2} \cdot \operatorname{erfc}\left(-\frac{\phi - d_D}{w_D}\right) \quad (203)$$

```

pdbSet Silicon SPER PhaseTransWidth {<n>} ;# w_T (um)
pdbSet Silicon SPER DriftWidth {<n>} ;# w_D (um)
pdbSet Silicon SPER DriftFactor {<expression>} ;# f_D (unitless)
pdbSet Silicon SPER DriftDistance {<n>} ;# d_D (um)
pdbSet Silicon SPER SurfaceDriftProbability {<n>} ;# P (unitless)
pdbSet Silicon SPER DriftReductionLength ;# L_dr (um)
pdbSetDouble Silicon <dopant> SPER.DriftLength {<n>} ;# L_d (um)

```

The parameters `SurfaceDriftProbability` and `DriftReductionLength` can be specified for a specific dopant by:

```

pdbSetDouble Silicon <dopant> SPER.SurfaceDriftProbability {<n>}
pdbSetDouble Silicon <dopant> SPER.DriftReductionLength {<n>}

```

To control the clustering rate in the region between amorphous and crystalline regions, an additional term can be defined by:

```

pdbSetString Si <cluster> SPERBoundaryTerm {<expression>}
pdbSetString Si <dopant> SPERBoundaryTerm {<expression>}

```

**NOTE** The term added by `SPERBoundaryTerm` of `<cluster>` must be correctly subtracted by `SPERBoundaryTerm` of `<dopant>` so that the total dose conservation is kept, for example:

```

pdbSetString Si As3 SPERBoundaryTerm "-1e1*(0.99*AsTotal-3.0*As3)"
pdbSetString Si Arsenic SPERBoundaryTerm "3e1*(0.99*AsTotal-3.0*As3)"

```

The full equation of a dopant is described by:

$$\begin{aligned}
 \frac{\partial X}{\partial t} &= (1 - \alpha) \left. \frac{\partial X}{\partial t} \right|_{crystal} \\
 &+ \alpha \vec{\nabla} \cdot \left( D_{amor} \vec{\nabla} X \right) + \vec{\nabla} \cdot \left( f_D \alpha v_D L_d \left( 1 - (1 - P) \exp\left(-\frac{d}{L_{dr}}\right) \right) X \vec{\nabla} \alpha_s \right) - R \cdot \exp\left(-\frac{9\phi^2}{W_T^2}\right)
 \end{aligned} \quad (204)$$

where  $R$  is defined by `SPERBoundaryTerm`.

The maximum time step during SPER is set by:

$$\Delta t_{max} = \min(\text{SPER.TimeStepScale} \cdot \frac{W_T}{\max(v)}, \text{SPER.MaxTimeStep}) \quad (205)$$

#### 4: Diffusion

##### Solid Phase Epitaxial Regrowth Model

---

## Phase Field Method

Since the level-set method requires Cartesian grids to calculate the distance field, it may cause instability from the difficult time-step control as well as the interpolation error due to the decoupled method with the different mesh structure. The phase field method uses a consistent mesh structure, so that the phase and the other solutions are coupled seamlessly into the hydrodynamic Scharfetter–Gummel discretization scheme, which improves the convergence if there is high drift due to an abrupt phase change.

The phase field method solves the equation for the phase field  $\varphi$ , which is named with `SPERPhase`:

$$\tau \frac{\partial \varphi}{\partial t} = w^2 \nabla^2 \varphi - (\varphi^2 - 1)(\varphi - \lambda(\varphi^2 - 1)) \quad (206)$$

where:

- $\tau$ ,  $w$ , and  $\varphi$  are the relaxation time, the phase transition width, and the phase (-1 for completely amorphous, 1 for completely crystalline), respectively.
- $w$  and  $\lambda$  are given by the parameters `PhaseTransWidth` and `Lambda.Fac`, respectively.

The inverse of the relaxation time  $\tau$  is calculated by:

$$\tau^{-1} = f_{iso} f_{aniso} R \exp\left(-\frac{E_{aniso} + E_{Sv} + E_{Ss}}{kT}\right) \quad (207)$$

where:

- $f_{iso}$  and  $f_{aniso}$  are the isotropic and anisotropic multiplication factors, respectively.
- $R$  is the relaxation rate.
- $E_{aniso}$ ,  $E_{Sv}$  and  $E_{Ss}$  are the orientation-dependent, the hydrostatic stress-dependent, and shear stress-dependent activation energies, respectively.

$$E_{aniso} = \sum_{100, 110, 111} E.Aniso \cdot \frac{\nabla \varphi}{\|\nabla \varphi\|} \quad (208)$$

$$E_{Sv} = P \cdot VFreeCrys \quad (209)$$

$$E_{Ss} = \text{Shear.Coupling} \cdot (|\epsilon_{xy}| + |\epsilon_{yz}| + |\epsilon_{zx}|) \quad (210)$$

```
pdbSet Silicon SPER Relax.Rate {<n>} ;# R(1/s)
pdbSet Silicon SPER R.Fac {<expression>} ;# f_iso (unitless)
pdbSet Silicon SPER R.Fac.Aniso {100 <n> 110 <n> 111 <n>} ;# f_aniso (unitless)
pdbSet Silicon SPER E.Aniso {100 <n> 110 <n> 111 <n>} ;# E_aniso (eV)
```

```

pdbSet Silicon SPER VFrecrys {<n>} ;# (cm-3)
pdbSet Silicon SPER Shear.Coupling {<n>} ;# (eV)

```

The phase field method assumes no diffusion in a crystalline region during SPER, so that the diffusion equation of a dopant is formulated by:

$$\frac{\partial X}{\partial t} = \left(\frac{1-\varphi}{2}\right) \vec{\nabla} \cdot \left( D_{amor} \vec{\nabla} X + D_{amor} X \frac{E_{seg}}{kT} \vec{\nabla} \varphi \right) \quad (211)$$

where  $E_{seg}$  is the chemical potential energy difference to cause the dopant segregation at an amorphous–crystalline boundary.

$E_{seg}$  is given by the parameter `SPER.Energy` that you can define with a string expression:

```

pdbSet Silicon <dopant> SPER.Energy {<expression>} ;# E_seg (eV)

```

The maximum time step during SPER is set by:

$$\Delta t_{max} = \min(\text{SPER.TimeStepScale} \cdot \frac{\tau_{min}}{4}, \text{SPER.MaxTimeStep}) \quad (212)$$

As soon as regrowth is completed, the dopant activation in the regrowth region is performed with the `pdb` parameter `AmInit` or the term  `${Sol}AmInit`.

**NOTE** Since the dopant active concentration is initialized after regrowth is completed, the evaluated values of some terms, such as  `${Sol}Total` and  `${Sol}Active` can be incorrect during SPER.

## Flash or Laser Anneal Model

The flash or laser anneal model becomes necessary for an advanced process that requires diffusionless, but high activation. The model can simulate the inhomogeneous thermal distribution, which results in better accuracy for stress calculation as well as heat transfer delay to the region in which the devices form.

The solution name of the local temperature  $T$  (in kelvin) is `Temperature`. The model is switched on by specifying the Boolean parameter `laser` in a diffusion statement. For example:

```

diffuse temperature=500 time=1<ms> laser

```

For a melting laser anneal, the phase field variable  $\varphi$  is introduced to describe whether the material is liquid or solid. The solution name of the phase  $\varphi$  is `HeatPhase`. The melting laser anneal model is invoked by switching on the Boolean parameter `Use.Melting.Laser`:

```

pdbSet Heat Use.Melting.Laser 1

```

#### 4: Diffusion

Flash or Laser Anneal Model

---

## Heat Transfer Equation

The heat transfer equation is:

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (\kappa \nabla T) + G + 30\rho L \varphi^2 (1 - \varphi)^2 \frac{\partial \varphi}{\partial t} \quad (213)$$

where:

- $\kappa$ ,  $\rho$ , and  $c_p$  are the conductivity, the mass density, and the specific heat capacity, respectively.  $\kappa$  and  $c_p$  can depend on temperature.
- $L$  is the unit mass latent heat (Eq. 244). The phase-dependent term takes the heat consumption (or generation) due to the solid-to-liquid (or liquid-to-solid) phase change into account.

$c_p$  and  $\kappa$  vary with the liquid, or amorphous, or crystalline phase as follows:

$$c_p = \varphi(\alpha c_{pa} + (1 - \alpha)c_{pc}) + (1 - \varphi)c_{pl} \quad (214)$$

$$\kappa = \varphi(\alpha \kappa_a + (1 - \alpha)\kappa_c) + (1 - \varphi)\kappa_l \quad (215)$$

where the subscripts  $a$ ,  $c$ , and  $l$  of  $c_p$  and  $\kappa$  indicate the amorphous phase, the crystalline phase, and the liquid phase, respectively. The  $\alpha$  is the degree of the structural disorder in a material that is calculated by:

$$\alpha = \frac{1}{2} \left( 1 + \tanh \left( 10 \ln \left( \frac{D_{FP}}{D_{max}} \right) \right) \right) \quad (216)$$

where  $D_{FP}$  is the Frenkel pair concentration by implantation damage, and  $D_{max}$  is the amorphous threshold to determine the amorphous and crystal transition:

```
 pdbSet <material> SpecificHeatCapacity {<expression>}      ;# Cpc (J/kg/K)
 pdbSet <material> Amorphous.SpecificHeatCapacity {<expression>} ;# Cpa (J/kg/K)
 pdbSet <material> Liquid.SpecificHeatCapacity {<expression>}   ;# Cpl (J/kg/K)
 pdbSet <material> ThermalConductivity {<expression>}          ;# kc (W/cm/K)
 pdbSet <material> Amorphous.ThermalConductivity {<expression>} ;# ka (W/cm/K)
 pdbSet <material> Liquid.ThermalConductivity {<expression>}    ;# kl (W/cm/K)
```

The heat generation rate  $G$  is calculated by:

$$G = I_0 \cdot g \quad (217)$$

where  $I_0$  and  $g$  represent the given intensity and the normalized profile, respectively. See [Intensity Models for Flash Anneal on page 217](#) and [Intensity Model for Scanning Laser on page 219](#) for the intensity models of  $I_0$ .

The normalized profile is calculated by one of the following methods:

- Energy implantation method (the default) (see [Energy Implantation Method](#))
- Transfer matrix method (see [Transfer Matrix Method](#))
- Finite-difference time-domain method (see [Finite-Difference Time-Domain Method on page 207](#))

## Energy Implantation Method

The energy implantation method (EIM) assumes conservation of energy dose and no reflection at material interfaces. EIM applies only to 1D and 2D structure simulations. To calculate the heat generation with EIM, use:

```
pdbSet Heat Heat.Rate.Model EIM
```

The implantation profile is generated as follows:

- The first moment is zero, so that the peak value of the distribution in each region is located at the surface of the region.
- The lateral decay length is given by `HeatLateralDecayLength`, that is:

```
pdbSet <mat> HeatLateralDecayLength <n> ;# cm (default: 1e-6)
```

- The normalized distribution is  $g$  of which the integration along the light path is 1.0:

$$g = \alpha \exp\left(-\int_{l=0}^{l=d} \alpha dl\right) \quad (218)$$

where  $\alpha$  is the absorption coefficient, which is given by the user-defined expression:

```
pdbSet <material> Absorptivity {<expression>} ;# cm-1
```

## Transfer Matrix Method

The transfer matrix method (TMM) calculates the reflectance, transmittance, and absorbance for both parallel and perpendicular polarizations. The monochromatic plane waves with arbitrary angles of incidence and polarization states penetrating a number of planar, parallel layers are assumed. TMM applies only to 1D and 2D structure simulations. To calculate the heat generation with TMM, use:

```
pdbSet Heat Heat.Rate.Model TMM
```

**NOTE** For backward compatibility with releases prior to Version L-2016.03, when you switch on `Use.TMM`, TMM will be used regardless of the specification of `Heat.Rate.Model`.

## 4: Diffusion

### Flash or Laser Anneal Model

The 2D simulation structure is split into multiple vertical segments. The boundary of each region is traced and evaluated for a change of the edge direction. When the edge direction is changed more than the given criterion `Minimum.Angle.Between.Segments`, the region is split unless the width of the segment is narrower than the given criterion `Minimum.Segment.Width`. An identical layer stack is assumed within each vertical segment. The TMM solver calculates the heat generation rate per each vertical segment:

```
pdbSet Heat Minimum.Angle.Between.Segments <n> ;# degree (default: 8.11)
pdbSet Heat Minimum.Segment.Width <n> ;# cm (default: 1E-7)
```

Each layer must be homogeneous, isotropic, and optically linear. In this case, the amplitudes of the forward and backward running waves  $A_j^\pm$  and  $B_j^\pm$  in each layer in [Figure 20 on page 206](#) are calculated with the help of transfer matrices. These matrices are functions of the complex wave impedances  $Z_j$  given by:

- $Z_j = \tilde{n}_j \cdot \cos\Theta_j$  in the case of E polarization (TE).
- $Z_j = \tilde{n}_j / (\cos\Theta_j)$  in the case of H polarization (TM).

Here,  $\tilde{n}_j$  denotes the complex index of refraction and  $\Theta_j$  is the complex counterpart of the angle of refraction ( $\tilde{n}_0 \cdot \sin\Theta_0 = \tilde{n}_j \cdot \sin\Theta_j$ ). The incidence angle  $\Theta_0$ , which is the angle of incident light to the vertical axis (the x-axis in the unified coordinate system (UCS)), is given by:

```
pdbSet Heat Incidence.Polar.Angle <n> ;# degree (default: 0.0)
```

The complex refractive index (CRI)  $\tilde{n}$  can be written as:

$$\tilde{n} = n + i \cdot k \quad (219)$$

with:

$$n = n_0(\lambda) + \Delta n_T \quad (220)$$

where  $\lambda$  is the wavelength of the incident light. The real part  $n$  is composed of the wavelength-dependent refractive index  $n_0$  and the correction terms  $\Delta n_T$  for the dependency on temperature:

$$\Delta n_T = n_T \cdot (T - T_{\text{npar}}) \quad (221)$$

where  $n_0$ ,  $n_T$ , and  $T_{\text{npar}}$  are given by:

```
pdbSet <mat> Refractive.Index {<\lambda_1> <n_1> ... <\lambda_m> <n_m>} ;# wavelength (nm)
pdbSet <mat> Refractive.Index.T0 <n>
pdbSet <mat> Refractive.Index.Tpar <n>
```

The imaginary part  $k$  is composed of the wavelength-dependent extinction coefficient  $k_0$  and the temperature-dependent factor:

$$k = k_0(\lambda) \cdot \exp(k_T \cdot (T - T_{\text{kpar}})) \quad (222)$$

where  $k_0$ ,  $k_T$ , and  $T_{\text{kpar}}$  are given by:

```

pdbSet <mat> Extinction.Coeff {<λ₁> <k₁> ... <λₘ> <kₘ>} ;# wavelength (nm)
pdbSet <mat> Extinction.Coeff.T0 <n>
pdbSet <mat> Extinction.Coeff.Tpar <n>

```

**NOTE** The TMM assumes a constant CRI in the same material region at a given global temperature.

The absorption coefficient  $\alpha$  is computed from  $k$  and  $\lambda$  according to:

$$\alpha = \frac{4\pi}{\lambda} \cdot k \quad (223)$$

The transfer matrix of the interface between layers  $j$  and  $j + 1$  is defined by:

$$T_{j,j+1} = \frac{1}{2Z_j} \cdot \begin{bmatrix} Z_j + Z_{j+1} & Z_j - Z_{j+1} \\ Z_j - Z_{j+1} & Z_j + Z_{j+1} \end{bmatrix} \quad (224)$$

The propagation of the plane waves through layer  $j$  can be described by the transfer matrix:

$$T_j(d_j) = \begin{bmatrix} \exp\left(2\pi i n_j \cos \Theta_j \frac{d_j}{\lambda}\right) & 0 \\ 0 & \exp\left(-2\pi i n_j \cos \Theta_j \frac{d_j}{\lambda}\right) \end{bmatrix} \quad (225)$$

with the thickness  $d_j$  of layer  $j$ .

The transfer matrices connect the amplitudes of [Figure 20 on page 206](#) as follows:

$$\begin{aligned}
 \begin{bmatrix} B_j^+ \\ A_j^+ \end{bmatrix} &= T_{j,j+1} \cdot \begin{bmatrix} A_{j+1}^- \\ B_{j+1}^- \end{bmatrix} \\
 \begin{bmatrix} A_j^- \\ B_j^- \end{bmatrix} &= T_j(d_j) \cdot \begin{bmatrix} B_j^+ \\ A_j^+ \end{bmatrix}
 \end{aligned} \quad (226)$$

#### 4: Diffusion

##### Flash or Laser Anneal Model

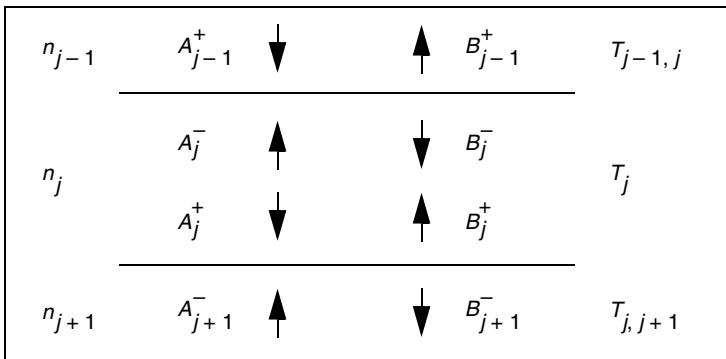


Figure 20 Wave amplitudes in a layered medium and transfer matrices connecting them

It is assumed that there is no backward-running wave behind the layered medium, and the intensity of the incident radiation is known. Therefore, the amplitudes  $A_j^\pm$  and  $B_j^\pm$  at each interface can be calculated with appropriate products of the transfer matrices.

For both cases of polarization, the intensity in layer  $j$  at a distance  $d$  from the upper interface ( $j, j + 1$ ) is given by:

$$I_{T(\text{TE, TM})}(d) = \frac{\Re(Z_j)}{\Re(Z_0)} \cdot \left\| T_j(d) \cdot \begin{pmatrix} A_j^- \\ B_j^- \end{pmatrix} \right\|^2 \quad (227)$$

with the proper wave impedances. If  $\delta$  is the angle between the vector of the electric field and the plane of incidence, the intensities must be added according to:

$$I(d) = I_{\text{TM}}(d) + I_{\text{TE}}(d) \quad (228)$$

where  $I_{\text{TM}} = (1 - a)I(d)$  and  $I_{\text{TE}} = aI(d)$  with  $a = \cos^2 \delta$ .

The polarization angle  $\delta$  is given by:

```
pdbSet Heat Polarization.Angle <n> ;# degree (default: 45)
```

The absorption coefficient  $\alpha$  is the relative rate of decrease in the light intensity along its path of propagation due to absorption. This decrease must be distinguished from variations caused by the superposition of waves. Therefore, the normalized heat generation rate is:

$$g = \alpha \frac{I(d)}{I_0} \quad (229)$$

## Finite-Difference Time-Domain Method

**NOTE** You must have licenses for Sentaurus Mesh and Sentaurus Device Electromagnetic Wave Solver (EMW) to use this method.

The finite-difference time-domain (FDTD) method is the most accurate method for complex structures. It executes EMW to calculate the heat generation rate. To calculate the heat generation rate using the FDTD method, specify:

```
pdbSet Heat Heat.Rate.Model EMW
```

To generate the correct tensor mesh structure for this solver, the FDTD method executes Sentaurus Mesh. The FDTD method applies only to 2D and 3D structure simulations.

The TMM and the FDTD method share PDB parameters such as the complex refractive index (CRI), the incidence angles, and the polarization angle, as well as the temperature-dependent CRI model (see [Eq. 219–Eq. 222](#)). The following parameters are shared:

```
pdbSet Heat Polarization.Angle <n> ;# degree (default: 45)
pdbSet Heat Incidence.Polar.Angle <n> ;# degree (default: 0.0)

pdbSet <mat> Refractive.Index {<λ1> <n1> ... <λm> <nm>} ;# wavelength (nm)
pdbSet <mat> Extinction.Coeff {<λ1> <k1> ... <λm> <km>} ;# wavelength (nm)
pdbSet <mat> Refractive.Index.T0 <n>
pdbSet <mat> Refractive.Index.Tpar <n>
pdbSet <mat> Extinction.Coeff.T0 <n>
pdbSet <mat> Extinction.Coeff.Tpar <n>
```

However, for [Eq. 221](#) and [Eq. 222](#), a local temperature is used in the FDTD method, while a global temperature is used in TMM. In the FDTD method, the CRI in amorphous or liquid regions can be specified to different values from that of the crystal region. The following parameters are available only for the FDTD method:

```
pdbSet Heat Incidence.Azimuthal.Angle <n>

pdbSet <mat> Liquid.Refractive.Index {<λ1> <n1> ... <λm> <nm>}
pdbSet <mat> Liquid.Extinction.Coeff {<λ1> <n1> ... <λm> <nm>}
pdbSet <mat> Liquid.Refractive.Index.T0 <n> ;# default 0.0 1/K
pdbSet <mat> Liquid.Refractive.Index.Tpar <n> ;# default 300.0 K
pdbSet <mat> Liquid.Extinction.Coeff.T0 <n> ;# default 0.0 1/K
pdbSet <mat> Liquid.Extinction.Coeff.Tpar <n> ;# default 300.0 K

pdbSet <mat> Amorphous.Refractive.Index {<λ1> <n1> ... <λm> <nm>}
pdbSet <mat> Amorphous.Extinction.Coeff {<λ1> <n1> ... <λm> <nm>}
pdbSet <mat> Amorphous.Refractive.Index.T0 <n> ;#def. Refractive.Index.T0
pdbSet <mat> Amorphous.Refractive.Index.Tpar <n> ;#def. Refractive.Index.Tpar
pdbSet <mat> Amorphous.Extinction.Coeff.T0 <n> ;#def. Extinction.Coeff.T0
pdbSet <mat> Amorphous.Extinction.Coeff.Tpar <n> ;#def. Extinction.Coeff.Tpar
```

#### 4: Diffusion

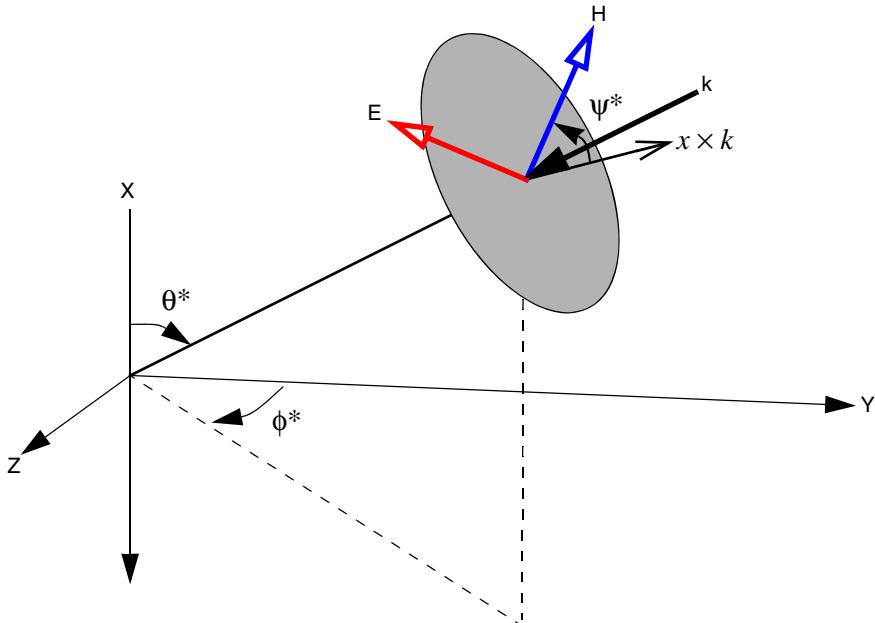
##### Flash or Laser Anneal Model

In EMW, the propagation direction is defined by the `Incidence.Polar.Angle` ( $\theta^*$ ) parameter and the `Incidence.Azimuthal.Angle` ( $\phi^*$ ) parameter, which denote the angles in degrees from the  $-x$ -axis and  $y$ -axis, respectively (see [Figure 21](#)). The parameter `Incidence.Azimuthal.Angle` is the angle to the horizontal axis (the  $y$ -axis in the UCS) and applies only to 3D simulations. It is set to zero for 2D simulations.

In addition, the parameter `Polarization.Angle` ( $\psi^*$ ) is used to set the polarization angle, which is measured from the  $x \times \hat{k}$  axis (see [Figure 21](#)). In this definition:

- `Polarization.Angle = 90°` and `Polarization.Angle = 270°` correspond to TE polarization.
- `Polarization.Angle = 0°` and `Polarization.Angle = 180°` correspond to TM polarization.

**NOTE** Before passing the excitation angles  $\theta^*$ ,  $\phi^*$ , and  $\psi^*$  to EMW, the angles are converted to comply with the definition of EMW.



**Figure 21** Definition of coordinate system for 3D plane wave excitation and examples of parameters of 3D plane wave:  $\theta^*$ ,  $\phi^*$ , and  $\psi^*$  are the `Incidence.Polar.Angle`, `Azimuthal.Angle`, and `Polarization.Angle`, respectively

The refractive index and the extinction coefficient are calculated by:

$$n(\varphi, \alpha, T) = \varphi((1 - \alpha)n_c(T) + \alpha n_a(T)) + (1 - \varphi)n_l(T) \quad (230)$$

$$k(\varphi, \alpha, T) = \varphi((1 - \alpha)k_c(T) + \alpha k_a(T)) + (1 - \varphi)k_l(T) \quad (231)$$

where  $\varphi$ ,  $\alpha$ , and  $T$  are the solid phase, the degree of structural disorder, and the local temperature, respectively.

$$n(T) = n(T_{\text{npar}}) + T_{n0}(T - T_{\text{npar}}) \quad \text{for } n_c, n_a, \text{ and } n_l \quad (232)$$

$$k(T) = k(T_{\text{kpar}}) \exp(T_{k0}(T - T_{\text{kpar}})) \quad \text{for } k_c, k_a, \text{ and } k_l \quad (233)$$

If  $n(T_{\text{npar}})$  and  $k(T_{\text{kpar}})$  for liquid and amorphous regions are not specified, the values of a crystalline material are used. The FDTD method generates the tensor-mesh structure by setting the maximum cell size  $\Delta x$  to Eq. 234 in each material region:

$$\Delta x = \frac{\lambda}{\max(\sqrt{n^2 + k^2})} / \text{Nodes.Per.Wavelength} \quad (234)$$

However, if you want to control more details such as a denser mesh near the interface, you may want to directly write the Sentaurus Mesh command file. In that case, you must include the following section in the command file:

```
IOControls {
    inputFile= "@inputfile@"
    outputFile= "@outputfile@"
}
```

In addition, you must define `EMW.Mesh.Template` to the name of the Sentaurus Mesh command file, for example, `smesh.template`, as follows:

```
pdbSet Heat EMW.Mesh.Template smesh.template
```

To run EMW, the FDTD method generates the command file from the template file provided by users. The template file for the command file of EMW must include the following sections:

```
Global {
    FieldDataFile= "@fielddatafile@"
    GridFile= "@gridfile@"
   LogFile= "@logfile@"
    ResultFile= "@resultfile@"
}

PlaneWaveExcitation {
    BoxCorner1= @boxcorner1@
    BoxCorner2= @boxcorner2@
    Wavelength= @wavelength@
    Psi=@psi@
    Theta=@theta@
    Phi=@phi@
    Intensity=@intensity@
}
```

## 4: Diffusion

### Flash or Laser Anneal Model

```
Extractor {
    Name= "@extname@"
    Quantity= { AbsorbedPhotonDensity }
    GridFile= "@extgridfile@"
}
```

**NOTE** The excitation angles @theta@, @phi@, and @psi@ refer to the angles  $\theta^*$ ,  $\phi^*$ , and  $\psi^*$  as defined in [Figure 21 on page 208](#).

Since the FDTD method runs Sentaurus Mesh and EMW, temporary files are generated for communication between the tools and these files are cleaned up after communication. If you want to keep the temporary files for debugging purposes, switch on the following parameter:

```
pdbSet Heat EMW.Keep.Temporary.Files 1 ;# default 0
```

Since the CRI varies with temperature and the thermodynamic phase such as crystallinity and solid phase, the normalized heat rate  $g$  must be recalculated when the CRI changes. The recalculation at every internal diffusion step can be forced by:

```
pdbSet Heat UpdateHeatRate 1
```

However, running EMW at each step takes a long time even for a single diffusion command. Therefore, it is better to update the normalized heat rate  $g$  only when the CRI change is not negligible. Such a criterion to run EMW with the updated CRI can be specified by:

```
pdbSet Heat Retrace.CRI.Change <n>
```

The normalized heat rate  $g$  is recalculated when:

$$\max(|(n - n')/n|) > \text{Retrace.CRI.Change} \quad (235)$$

or:

$$\max(|(k - k')/k|) > \text{Retrace.CRI.Change} \quad (236)$$

where  $n'$  is the previously stored refractive index, and  $k'$  is the previously stored extinction coefficient.

In addition to the CRI change criterion, you can force to continue the simulation without running EMW when the time step from the previous CRI update is shorter than Min.Time.Step.CRI.Change. This criterion takes precedence over the Retrace.CRI.Change criterion:

```
pdbSet Heat Min.Time.Step.CRI.Change <n> ;# unit=seconds, default= 1E-11
```

## Melting Phase Field Equation

The governing equation of the phase field  $\varphi$  is given by:

$$\frac{\partial \varphi}{\partial t} = \mu \gamma \nabla^2 \varphi - \frac{\mu \gamma}{\delta^2} \varphi (1 - \varphi) (1 - 2\varphi) + 5 \frac{v_{int}}{\delta} \varphi^2 (1 - \varphi)^2 + s(T, \varphi) \quad (237)$$

where:

- $\mu$ ,  $\gamma$ , and  $\delta$  are the melting interface mobility, the surface tension, and the interface thickness, respectively.  $\mu$  and  $\gamma$  depend on material crystallinity.
- $s(T, \varphi)$  is the seed function to start melting.
- $v_{int}$  is the interface response function to describe the front moving velocity of the flat melting interface:

$$\mu = \alpha \mu_a + (1 - \alpha) \mu_c \quad (238)$$

$$\gamma = \alpha \gamma_a + (1 - \alpha) \gamma_c \quad (239)$$

```

pdbSet <material> Melting.Interface.Mobility {<n>}           ;# uc (cm4/J/sec)
pdbSet <material> Amorphous.Melting.Interface.Mobility {<n>} ;# ua (cm4/J/sec)
pdbSet <material> Surface.Tension {<n>}                      ;# gammac (J/cm2)
pdbSet <material> Amorphous.Surface.Tension {<n>}            ;# gammaaa (J/cm2)
pdbSet <material> AmorpDensity {<n>}                          ;# Dmax (cm-3)

```

The seed function is modeled by:

$$s(T, \varphi) = -f_s \frac{\mu \gamma}{\delta^2} \varphi \left( 1 - \frac{1}{2} \operatorname{erfc} \left( \frac{T - T_m}{T_s} \right) \right) \quad (240)$$

where  $T_m$  is the melting point.  $f_s$  and  $T_s$  are the multiplier and the temperature to control initial melting. The seed term in Eq. 237 is switched off when  $\varphi$  is reduced to less than the SeedOffPhase value:

```

pdbSet Heat Seed.Factor {<expression>}    ;# fs (unitless)
pdbSet Heat Seed.Temperature {<n>}         ;# Ts (K)
pdbSet Heat SeedOffPhase {<n>}              ;# unitless

```

It is known that the melting point varies with the dopant concentration, such as for germanium, as well as material crystallinity. The melting point is calculated by:

$$T_m = \alpha \left( T_{ma0} + (T_{ma1} - T_{ma0}) \frac{C_x}{C_{max}} \right) + (1 - \alpha) \left( T_{mc0} + (T_{mc1} - T_{mc0}) \frac{C_x}{C_{max}} \right) \quad (241)$$

#### 4: Diffusion

##### Flash or Laser Anneal Model

where  $\alpha$ ,  $T_{ma0}$ , and  $T_{mc0}$  are the degree of structural disorder, and the melting point of amorphous material and crystalline material, respectively.  $C_x$  is the concentration of the dopant that affects the melting point. For example:

```

pdbSet Silicon Melting.Point 1690 ;# Tmc0
pdbSet Silicon Amorphous.Melting.Point 1420 ;# Tma0
pdbSet Silicon Dop.Dep.Melting.Point { Ge { 960 1211 } } ;# Tmai and Tmc1

```

The interface response function  $V_{int}$  is modeled by the Frenkel–Wilson law [6]:

$$V_{int} = v \left( 1 - \exp\left(\frac{\rho L / C_{max}}{kT_m}(T - T_m)\right) \right) \quad (242)$$

where  $C_{max}$  is the lattice density. The liquid-to-solid interface transfer rate  $v$  is given by:

$$v = \begin{cases} v_0 \exp\left(-\frac{H}{kT}\right) & \text{for Arrhenius model} \\ v_{0f} \exp\left(-\frac{B}{k(T - T_g)}\right) & \text{for Vogel–Fulcher model} \end{cases} \quad (243)$$

where the model can be selected by:

```
pdbSet <material> Melting.Velocity.Model {Arrhenius | FulcherVogel}
```

The latent heat and the liquid-to-solid interface transfer rate depend on crystallinity as follows:

$$L = \alpha L_a + (1 - \alpha) L_c \quad (244)$$

$$v_0 = \alpha v_{0a} + (1 - \alpha) v_{0c} \quad (245)$$

$$H = \alpha H_a + (1 - \alpha) H_c \quad (246)$$

$$v_{0f} = \alpha v_{0fa} + (1 - \alpha) v_{0fc} \quad (247)$$

$$B = \alpha B_a + (1 - \alpha) B_c \quad (248)$$

$$T_{g0} = \alpha T_{ga} + (1 - \alpha) T_{gc} \quad (249)$$

where the subscripts  $a$  and  $c$  indicate the parameter for the amorphous and crystalline materials, respectively.

```

pdbSet <material> Latent.Heat {<n>} ;# Lc (J/kg)
pdbSet <material> Amorphous.Latent.Heat {<n>} ;# La (J/kg)
pdbSet <material> Melting.Velocity.0 {<n>} ;# v0c (cm/s)
pdbSet <material> Melting.Velocity.E {<n>} ;# Hc (eV)
pdbSet <material> Amorphous.Melting.Velocity.0 {<n>} ;# v0a (cm/s)

```

```

pdbSet <material> Amorphous.Melting.Velocity.E {<n>}      ;# Ha (eV)
pdbSet <material> FV.Melting.Velocity.0 {<n>}            ;# v0c (cm/s)
pdbSet <material> FV.Melting.Velocity.E {<n>}            ;# Hc (eV)
pdbSet <material> FV.Melting.Velocity.T {<n>}            ;# Tgc (K)
pdbSet <material> FV.Amorphous.Melting.Velocity.0 {<n>} ;# v0a (cm/s)
pdbSet <material> FV.Amorphous.Melting.Velocity.E {<n>} ;# Ha (eV)
pdbSet <material> FV.Amorphous.Melting.Velocity.T {<n>} ;# Tga (K)

```

---

## Crystallinity Phase Field Equation

When an amorphous region is molten and solidified, its crystallinity depends on the cooling rate. It is assumed that the cooling rate is small enough to fully crystallize the solidified region. The crystallinity phase field is updated by solving the equation:

$$\Delta\alpha = -\alpha \left( 1 - \frac{1}{2} \operatorname{erfc} \left( \log \left( \frac{\varphi_{\text{rec}}}{\varphi + \varepsilon \varphi_{\text{rec}}} \right) \right) \right) \quad (250)$$

where:

- $\Delta\alpha$  is the change of crystallinity per time step.
- $\varphi_{\text{rec}}$  is the parameter to control which melting status begins to lose crystallinity information.
- $\varepsilon$  is a scaling factor of  $\varphi_{\text{rec}}$  to avoid a zero denominator:

```

pdbSet Heat RecrystalOnPhase <n>          ;# default: 1E-2
pdbSet Heat Recrystal.Control.Factor <n>    ;# default: 1E-6

```

---

## Dopant Diffusion in Melting Laser Anneal

Since a melting or solidification process occurs too quickly to observe the dopant diffusion in a solid region, it is assumed that the dopant atoms diffuse only by entropic force and temperature gradient. The different chemical potentials of dopants at liquid, solid, and boundary regions induce the segregation. During melting laser anneal, the temperature varies greatly depending on the location.

Therefore, the dopant diffusion equation must be solved by coupling it to the heat equation ([Eq. 213, p. 202](#)) and the phase equation ([Eq. 237, p. 211](#)):

$$\frac{\partial C}{\partial t} = \nabla \cdot \left( D \frac{C_{eq}}{C_{eq0}} \nabla \left( C \frac{C_{eq0}}{C_{eq}} \right) \right) \quad (251)$$

## 4: Diffusion

### Flash or Laser Anneal Model

$$D = \begin{cases} D_{\text{liquid}} + (D_{\text{ils}} - D_{\text{liquid}}) \frac{\varphi}{\varphi_L} & \text{for } (\varphi \leq \varphi_L) \\ D_{\text{ils}} & \text{for } (\varphi_L < \varphi \leq \varphi_S) \\ D_{\text{solid}} + (D_{\text{ils}} - D_{\text{solid}}) \frac{1-\varphi}{1-\varphi_S} & \text{for } (\varphi_S \leq \varphi) \\ \varphi D_{\text{solid}} + (1-\varphi) D_{\text{liquid}} & \text{if } (\varphi_L > \varphi_S) \end{cases} \quad (252)$$

$$\frac{C_{eq}}{C_{eq0}} = \exp\left(-\frac{\varphi E_{\text{seg}} + 16\varphi^2(1-\varphi)^2 E_{\text{intf}}}{kT}\right) \quad (253)$$

where:

- $D_{\text{liquid}}$ ,  $D_{\text{ils}}$ , and  $D_{\text{solid}}$  are the dopant diffusivities in a liquid, a liquid–solid interface, and solid regions, respectively.  $D_{\text{solid}}$  is calculated by an Arrhenius formula with global temperature.
- $E_{\text{seg}}$  and  $E_{\text{intf}}$  are the chemical potential energies in a solid state and an interface state relative to that in a liquid state, respectively.

```

pdbSet Heat Max.Liquid.Phase {<n>} ;# phi_L (unitless)
pdbSet Heat Min.Solid.Phase {<n>} ;# phi_S (unitless)
pdbSet <material> <dopant> Dliquid.0 {<n>} ;# cm2/s
pdbSet <material> <dopant> Dliquid.E {<n>} ;# eV
pdbSet <material> <dopant> Dils.0 {<n>} ;# cm2/s
pdbSet <material> <dopant> Dils.E {<n>} ;# eV
pdbSet <material> <dopant> Dstar {<n>} ;# cm2/s (Dsolid)
pdbSet <material> <dopant> Melting.Seg.E {<n>} ;# eV
pdbSet <material> <dopant> Melting.Intf.Seg.E {<n>} ;# eV

```

To solve the dopant diffusion equation by coupling it with the heat and phase equations, use:

```

solution name= <dopant> ifpresent= <dopant> !negative Heat
pdbSetString <material> <dopant> InitHeatProc InitLiquidDopant
pdbSetString <material> <dopant> EquationHeatProc DopantLiquidBulk

```

By default, it is applied to boron, phosphorus, arsenic, antimony, and indium impurities.

The instant recrystallization of an amorphous region, that is, the initialization of cluster solutions, is performed before diffusion. The cluster solutions are reset to zero in a melted region during diffusion by multiplying  $\varphi$  by the cluster solutions, which implies that all dopants in a liquid region are activated fully. Like the cluster solutions, the point-defect and defect-cluster solutions are reset to zero in liquid regions.

## Parameter Setting Guidelines

The default value ( $1 \times 10^{-7}$  cm) of the `Heat . Phase . Width` variable (interface thickness  $\delta$ ) is typically good for simulating melting depths of  $\sim 100$  nm. For larger melting depths (such as  $1 \mu\text{m}$ ), a value of  $\sim 2 \times 10^{-7}$  cm can reduce the simulation time and still maintain reasonable accuracy:

```
pdbSet Si Heat.Phase.Width 1e-7 ;# cm
```

Mesh spacing in the molten region must always be smaller than `Heat . Phase . Width` ( $\delta$ ) to obtain proper convergence. A larger mesh spacing results in a faster simulation and less noise. Larger values of  $\delta$  can speed up convergence even for a fixed mesh spacing. The simulated dopant distribution depends on both mesh spacing and  $\delta$ . For an equidistant 1D mesh, the simulation results are almost the same for all mesh spacing  $< \delta$ . For an inhomogeneous 1D mesh, the simulated melting front speed changes when the solid–liquid interface reaches the region of mesh inhomogeneity, unless the maximum mesh spacing is smaller than  $\delta/8$ . A mesh finer than  $\delta/8$  may result in a larger CPU time. This basically means that mesh refinements are allowed only if the background mesh is finer than  $\delta/8$ . Therefore, an equidistant mesh should be used in the melting region whenever possible.

If mesh spacing is not smaller than the inverse of absorptivity ( $\alpha$ ), a numeric error appears in the expression for heat generation. The total integrated dose of scaled `HeatRate` is a good indicator of the presence of such an error, which can be checked in the output file. For example, for a 0.5-nm mesh and  $\alpha = 1.46 \times 10^6 \text{ cm}^{-1}$ , the scaled `HeatRate` dose equals  $1.0004 \times 10^{14}$ . The analytic total integrated `HeatRate` dose equals  $1.0 \times 10^{14}$ . A difference of more than  $1.0 \times 10^{-3}$  may cause a pronounced increase of the melting depth. Two solutions are possible:

- A finer mesh at the outer silicon interface. It may be limited by an increase of CPU time related to the mesh inhomogeneity constraint previously described.
- The laser fluence can be multiplied by the factor  $1.0 \times 10^{14}$  `TotalHeatRateDose`. This is performed automatically when `pdbSet Heat Correct.Energy.Dose 1` is applied. This option obtains good results at meshes when mesh spacing does not satisfy the criterion  $\text{mesh spacing} \ll 1/\alpha$ .

## Saving a Thermal Profile

To save the thermal profile computed during this step to a file, use the `write.temp.file` argument of the `diffuse` command. In a subsequent simulation, you can use this file to create a temperature ramp using the `read.temp.file` argument of the `temp_ramp` command. For more information, see [diffuse on page 935](#) and [temp\\_ramp on page 1224](#).

---

## Boundary Conditions

At the top surface, that is, the gas interface, the heat emission flux from the top material is given by:

$$F = -5.6703 \cdot 10^{-12} \cdot \text{Emissivity} \cdot (T^4 - T_0^4) \quad (254)$$

where  $T_0$  is the environment temperature specified by `temperature` in the `diffuse` command.

At the bottom, the boundary condition depends on whether the thermal resistor is attached. If `AttachThermalResistor` is switched on, the emission flux at bottom is calculated by:

$$F = -\left(\frac{\kappa}{t_w - x_{bot}}\right)(T - T_0) \quad (255)$$

where  $t_w$  and  $x_{bot}$  are the wafer thickness and the bottom coordinate of a simulation structure, respectively. Otherwise:

$$F = -\text{HeatSinkTransfer}(T - T_0) \quad (256)$$

The wafer thickness in micrometers is specified by:

```
pdbSet Heat WaferThickness <n>
```

At the sides, the flux is calculated by:

$$F = -\text{SideHeatTransfer}(T - T_0) \quad (257)$$

By default, `SideHeatTransfer` is set to zero for all materials.

---

## Structure Extension

The heat transfer is much faster in comparison with an impurity or a point-defect diffusion. For example, in silicon, the diffusion length of the heat temperature is 20–30 times longer than that of interstitials at 800°C. Therefore, solving the heat equation requires a much larger structure size than for diffusion equations. The model provides the method to temporarily extend the current structure for solving the heat equation, and then recovers the original structure after finishing the laser or flash anneal. The downward extension is controlled by the Boolean parameter `ExtendBottom`.

The location of the extended bottom is specified by `WaferThickness`, for example:

```
pdbSet Heat ExtendBottom 1  
pdbSet Heat WaferThickness 700
```

which are defined by default.

Since the flash light source transfers heat to the whole wafer surface at the same time, no heat flux is assumed at the structure sides so that you do not have to extend the structure along the side directions. However, since the laser anneal scans a wafer by beaming a laser on a localized spot, the structure must be extended to the side directions to correctly take into account the heat transfer from the beamed spot. The extended distance in micrometers to the sides is defined with:

```
pdbSet Heat SideExtension <n>
```

To reduce the computation time for the extension, one side among the left and right sides is extended first, and then the extended structure is reflected on the side that is defined by:

```
pdbSet Heat ReflectSide <Left | Right | None>
```

For example, the following statements specify an extension of 200 µm in the right direction and a reflection of the extended structure on the left side:

```
pdbSet Heat SideExtension 200  
pdbSet Heat ReflectSide Left
```

When `ReflectSide` is set to `None`, each side (that is, both the left and right sides) is extended.

The material of all the extended regions is set to `HeatSubstrate`. The thermal properties of the `HeatSubstrate` material are defined internally to the same as the `BulkMaterial` material (default value: Si). In the region of `HeatSubstrate`, only the heat equation is solved.

---

## Intensity Models for Flash Anneal

Intensity can be specified by a Gaussian model, a table lookup method, or a user-specified model:

```
pdbSet Heat Intensity.Model {Gaussian | Table | User}
```

#### 4: Diffusion

##### Flash or Laser Anneal Model

### Gaussian Model

The intensity  $I$  can be given by the Gaussian profile as follows:

$$I = \frac{\text{Fluence}}{\sqrt{2\pi}t_s} \exp\left(-\frac{(t-t_0)^2}{2t_s^2}\right) \quad (258)$$

$$t_s = \frac{\text{Pulse}}{2\sqrt{2\ln 2}} \quad (259)$$

where Pulse is the full width at half maximum (FWHM) time interval. The parameter Fluence is the energy dose in  $\text{J/cm}^2$ .

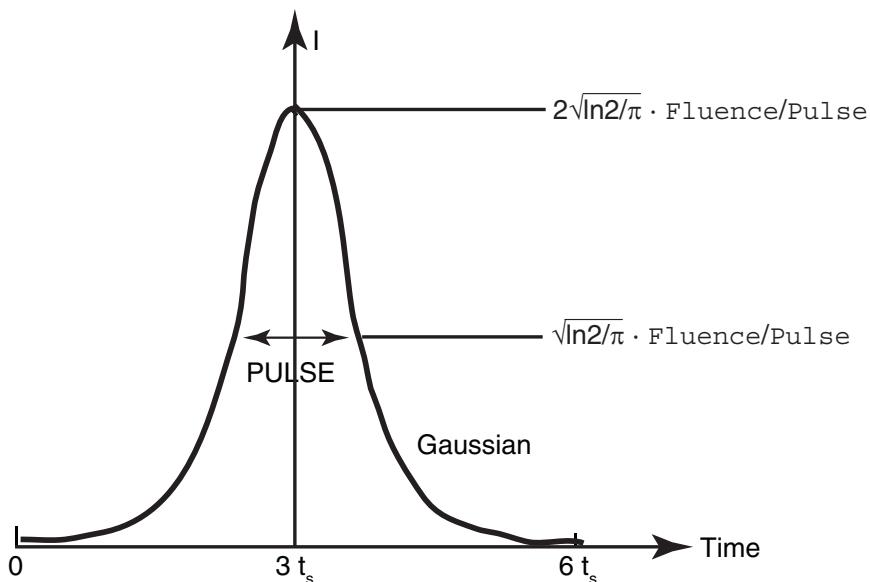


Figure 22 Heat Intensity for flash anneal with respect to time

### Table Lookup Method

The table of time versus intensity can be given by:

```
pdbSet Heat Intensity.Table { <t1> <I1> <t2> <I2> ... <tn> <In> }
```

The intensity values in the table can be scaled by:

```
pdbSet Heat Intensity.Table.Factor {<n>}
```

## User-Specified Model

You can define the heat intensity profile by using `IntensityProfile` (unit is  $\text{J/cm}^2/\text{s}$ ). The heating time, that is, the light-sourcing time for the user-specified intensity is given by the parameter `HeatingTime`. For example, for the sum of two different Gaussian intensities:

```
set ttime "\[simGetDouble Heat time\]"
set rt2pi [expr sqrt(2*3.141592)]
set tp1 3e-3 #from 3*sigma = 3*1e-3
set tp2 6e-3 #from 3*sigma = 3*2e-3
set ts1 2e-6 #from 2*sigma*sigma = 2*1e-3*1e-3
set ts2 8e-6 #from 2*sigma*sigma = 2*2e-3*2e-3

pdbSet Heat HeatingTime 12e-3
pdbSet Heat IntensityProfile "1e4/$rt2pi*exp(-(((ttime-$tp1)^2)/$ts1)) \
+2.5e3/$rt2pi*exp(-(((ttime-$tp2)^2)/$ts2))"
```

Here, `[simGetDouble Heat time]` returns the current time that is used to solve the heat equation.

---

## Intensity Model for Scanning Laser

The scanning laser beam is characterized with the scanning speed ( $\text{cm/s}$ ), the beam width ( $\mu\text{m}$ ), and the beam fading distance ( $\mu\text{m}$ ) by diffraction:

```
pdbSet Heat ScanSpeed <n>
pdbSet Heat BeamWidth <n>
pdbSet Heat BeamFadeDistance <n>
```

The intensity specification for laser beam precedents that of a flash light source. When a positive `ScanSpeed` is specified, the laser scanning model is assumed and the heat intensity is calculated with the laser beam parameters.

Two complementary error functions are multiplied to generate the laser beam intensity as shown in [Figure 23 on page 220](#).

#### 4: Diffusion

Flash or Laser Anneal Model

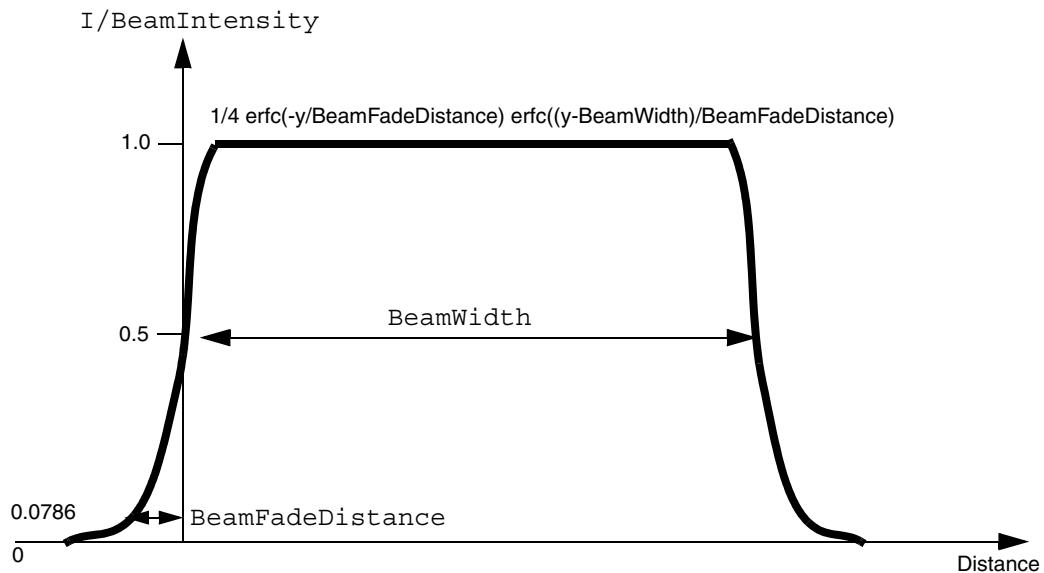


Figure 23 Heat intensity profile for laser beam

The laser beam moves by the distance ( $\text{BeamWidth}-\text{BeamOverlap}$ ) after  $(\text{BeamWidth}-\text{BeamOverlap})/\text{ScanSpeed}$  anneal time step. As  $\text{BeamOverlap}$  approaches  $\text{BeamWidth}$ , the simulation accuracy is improved.

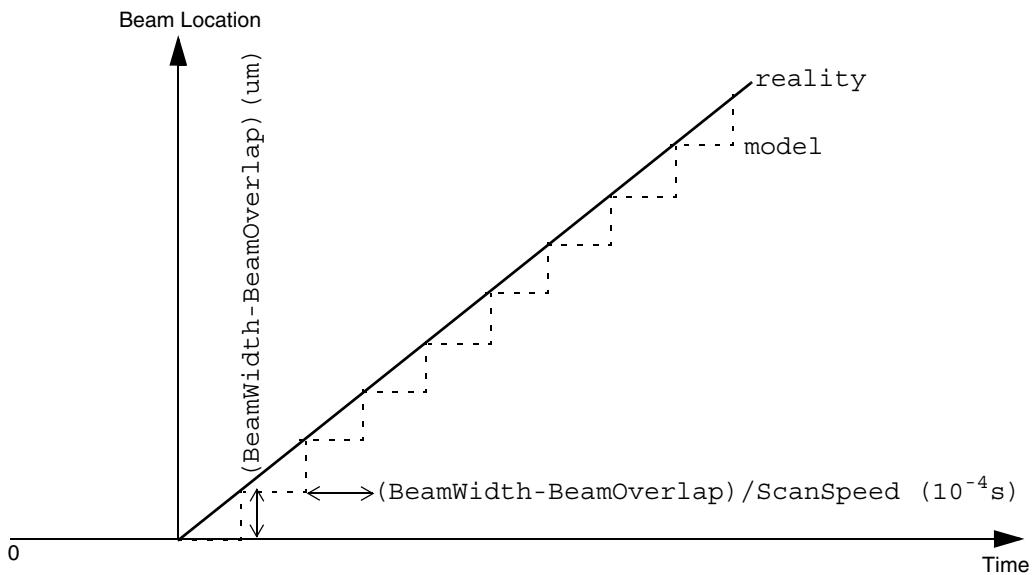


Figure 24 Beam location along time

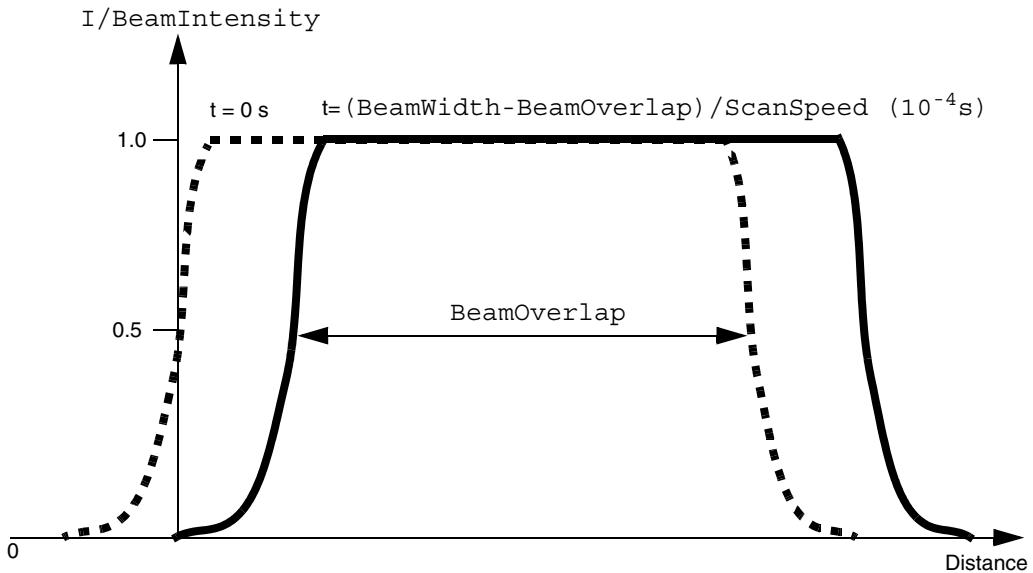


Figure 25 Laser beam displacement at each time step

## Control Parameters

[Table 14](#) lists the control parameters. These parameters must be used with:

`pdbSet Heat`

For example:

`pdbSet Heat HeatingTime 12e-3`

`pdbSet Heat MaxTimeStep 500`

Table 14 Control parameters

Parameter (with available options)	Default value Unit (if applicable)	Description
<code>AttachThermalResistor &lt;0   1&gt;</code>	0	Attaches the thermal resistor to the bottom. Options are 0   1.
<code>BulkMaterial &lt;material&gt;</code>	Si	Indicates that the global temperature for solving diffusion equations will be calculated by averaging the local temperatures at interfaces of the specified material. In addition, the material <code>HeatSubstrate</code> of the extended region will have the same thermal properties as <code>BulkMaterial</code> ones.

#### 4: Diffusion

Flash or Laser Anneal Model

Table 14 Control parameters

Parameter (with available options)	Default value Unit (if applicable)	Description
ExtendBottom <0   1>	1	Extends bottom of the simulation structure to the <b>WaferThickness</b> thickness. Options are 0   1.
HeatingTime <n>	0.0 ms	Defines the time the heating source is switched on. Not applicable to the scanning laser model.
HeatSinkTransfer <n>	1e5 W/(cm <sup>2</sup> K)	Defines the heat transfer rate coefficient at the extended structure bottom. Only applicable when <b>AttachThermalResistor</b> is set to 0.
MaxTimeStep <n>	600.0 s	Defines the maximum time step for solving the heat equation.
ReflectSide <Left   Right   None>	Left	Specifies the side at which the structure will be reflected after extending the structure to the other side by <b>SideExtension</b> . Only applicable for positive <b>SideExtension</b> . Options are Left   Right   None.
SideExtension <n>	0.0 μm	Defines the extended distance to side. The extended region is set to the <b>HeatSubstrate</b> material, which has the same thermal properties as the <b>BulkMaterial</b> ones. Note that only the heat equation is solved in the region of <b>HeatSubstrate</b> .
TempAverageBox "<x1,y1,z1,x2,y2,z2>"	-	Defines the box area to average the local temperatures for calculating the global temperature. It must be satisfied that $x1 \leq x2$ and $y1 \leq y2$ and $z1 \leq z2$ .  pdbSet Heat TempAverageBox "-0.1 0.1 0.0 1.0 2.0 0.0"
TimeSampleSize <n>	20.0	Specifies the number of time steps during the sourcing of the heat energy. Not applicable to the scanning laser model. The maximum time step is given by the minimum time step among <b>MaxTimeStep</b> and  $\frac{3 \cdot \text{Pulse}}{\text{TimeSampleSize} \cdot \sqrt{2 \ln 2}} \text{ (ms)}$ for $\text{HeatingTime} \leq 0.0$ , or $\text{HeatingTime}/\text{TimeSampleSize}$ .

Table 14 Control parameters

Parameter (with available options)	Default value Unit (if applicable)	Description
UpdateHeatRate <0   1>	0	Updates heat rate at each time step. Options are 0   1.
WaferThickness <n>	700.0 $\mu\text{m}$	Defines the wafer thickness to which the simulation structure is to be extended if ExtendBottom is set to 1.

## Notes

Notes are:

- It takes three times the standard deviation time to reach the peak intensity. After six times the standard deviation time, the heat source is switched off.
- The global temperature, which is calculated by averaging the local temperature distribution, is used to solve the diffusion equations.
- The global temperature is calculated by:

$$T_{global} = \frac{\sum_{i=1}^n V_i T_i}{\sum_{i=1}^n V_i} \quad (260)$$

where  $V_i$  and  $T_i$  are the volume and the local temperature at a node in BulkMaterial material. By default, the nodes on the nonreflecting surfaces of BulkMaterial are taken. When you set TempAverageBox, the nodes within the specified box are taken.

- By default, the global temperature is used to solve the mechanics equations. If you are interested in local temperature variation within the structure for mechanical analysis, you can use the following command before the laser annealing step:

```
pdbSetBoolean Mechanics UseTemperatureField 1
```

- When UseTemperatureField in mechanics is switched on, the local temperature is used to solve the mechanics equations. This PDB parameter must be used only for laser annealing and must be switched off after laser annealing. When this parameter is switched off, the local temperature must match the global temperature for accurate tracing of thermal stress history for the next process step.

## 4: Diffusion

### Diffusion in Polysilicon

---

## Diffusion in Polysilicon

Polysilicon has a microstructure composed of small monocrystalline grains of different crystalline orientation. The grains are separated by 2D surfaces – the grain boundaries.

Sentaurus Process uses a two-stream model to simulate polycrystalline or granular materials. Granular diffusion can be switched on with:

```
pdbSet PolySilicon Arsenic DiffModel Granular
```

---

## Isotropic Diffusion Model

The dopant concentration for species A is split into a fraction of dopants in the grain and a fraction of dopants in the grain boundary, that is:

$$C_A = f_g \cdot c_A^g + f_{gb} \cdot c_A^{gb} \quad (261)$$

Here,  $c_A^g$  denotes the total concentration inside the grain per grain volume and  $c_A^{gb}$  denotes the concentration inside the grain boundaries per grain boundary volume. Both quantities are defined in the entire polysilicon region representing average concentrations.

The ratio of grain volume to the polysilicon volume is known as the *volume share*. The volume share of the grain regions  $f_g$  depends on the shape and size of the grain. The volume share of the grain boundary is defined as:

$$f_{gb} = 1 - f_g \quad (262)$$

The grain volume share and grain boundary share are defined by the terms GVolShare and GbVolShare, respectively.

The concentration of the grain boundary is assumed to be electrically inactive. The grain density is identified with the active portion of the total concentration  $C_A^+$ . The active concentration is stored in the dataset <dopant>Active. The grain boundary concentration  $C_A^{gb} = f_{gb} \cdot c_A^{gb}$  is stored in the dataset <dopant>Gbc and is initialized with the portion of the total dopant concentration in the grain boundary  $f_{gb} \cdot C_A$ . In the absence of clusters, the total dopant concentration is given as:

$$C_A = f_g \cdot C_A^+ + C_A^{gb} \quad (263)$$

## Grain Shape and the Grain Growth Equation

The microscopic shape and size of the grains is not described in the model. Instead the size, orientation, and type of a prototype grain is used to compute all parameters that depend on the grain size.

The growth model can be switched on by:

```
pdbSet PolySilicon Dopant DiffModel Granular
```

In Sentaurus Process, a columnar grain structure is assumed by default. The grains are assumed to be columns that are oriented along the vertical axis, extending through the entire polycrystalline layer.

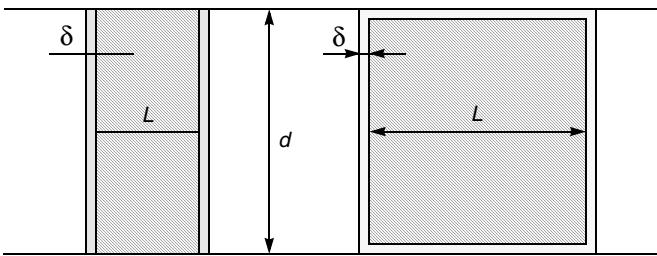


Figure 26 (Left) Columnar grains and (right) cubic grains:  $L$  is the grain size,  $\delta$  is the grain boundary thickness, and  $d$  is the layer thickness

The grain size  $L$  defines the average edge length of the square cross section of the columns. The grain size is stored in the dataset `GSize`. The volume share of the grain region is given as:

$$f_g = \left( \frac{L}{L + \delta} \right)^2 \quad (264)$$

For cubic grains, the volume share is:

$$f_g = \left( \frac{L}{L + \delta} \right)^3 \quad (265)$$

The grain shape and the initial values for the grain size  $L$  (cm) and grain boundary thickness  $\delta$  (cm) can be set in the parameter database, that is:

```
pdbSet PolySilicon GrainShape <model>
pdbSet PolySilicon GrainSize 5.0e-6
pdbSet PolySilicon GrainBoundaryThickness 5.0e-8
```

where `<model>` is either `Columnar` or `Cubic`. It is assumed that the layer thickness  $d$  is a constant value set as:

```
pdbSet PolySilicon LayerThickness 1.0e-6
```

## 4: Diffusion

### Diffusion in Polysilicon

The grains grow during thermal processes. During the grain growth, the volume share of the grains increases and the volume share of the grain boundary decreases. The grain growth is modeled by:

$$\frac{dL}{dt} = \frac{\tau^2 a_0 b_0^2 D \lambda}{kT} \cdot \frac{1}{1 + \frac{1}{a_r}} \cdot \left(1 - \frac{\sum c_{gb}}{C_{Si}}\right) \quad (266)$$

where  $a_r$  denotes the ratio between the grain boundary volume inside the polycrystalline layer and the grain boundary volume at the material interfaces of the polycrystalline layer bounding other materials. The grain size,  $L$ , is represented with the solution name `GSize` and can be monitored like other solution fields.

The grain growth parameters can be specified in the parameter database in the material entry. The following names are used:  $\tau$  Tau,  $\lambda$  Lambda, and  $a_0$  A0. The parameter  $b_0$  is twice the lattice spacing of silicon. The Arrhenius values for the various contributions to the silicon self-diffusivity  $D$  can be specified with the parameter `Dself`.

For columnar grains:

$$a_r = \frac{(2L + \delta)d}{2(L + \delta)^2} \quad (267)$$

$$\frac{dL}{dt} L \left(1 + \frac{2(L + \delta)^2}{(2L + \delta)d}\right) = \frac{\tau^2 a_0 b_0^2 D \lambda}{kT} \cdot \left(1 - \frac{\sum c_{gb}}{C_{Si}}\right) \quad (268)$$

For cubic grains, this is:

$$a_r = \frac{(3L^2 + 3L\delta + \delta^2)d}{2(L + \delta)^3} - \frac{1}{2} \quad (269)$$

$$\frac{dL}{dt} L \frac{d(3L^2 + 3L\delta + \delta^2) + (L + \delta)^3}{d(3L^2 + 3L\delta + \delta^2) - (L + \delta)^3} = \frac{\tau^2 a_0 b_0^2 D \lambda}{kT} \cdot \left(1 - \frac{\sum c_{gb}}{C_{Si}}\right) \quad (270)$$

The grain shape switches from `Cubic` to `Columnar` when the grain size  $L$  reaches the layer thickness  $d$  and the grain shape is set to `Cubic`, that is:

```
pdbSet PolySilicon GrainShape Cubic
```

This is the default. No switching is performed if the grain shape is set to `Columnar`. The grain growth equation is solved with the dopant diffusion equations.

Note that the `GSize` and the dopant distribution in the grain boundary `<dopant>Gbc` are not reset automatically at the beginning of a new diffusion step. The `pdb` switch `GbcNew` can be used to reset the grain size dataset `GSize` to the current value of `GrainSize`, that is:

```
pdbSet PolySilicon GrainSize 1e-6
pdbSet PolySilicon GbcNew 1
```

will reset the grain size in polysilicon to 10 nm. It also resets the `<dopant>Gbc` dataset to the value calculated using the grain size and the grain-boundary volume share.

The `GSize` and the initial `<dopant>Gbc` distribution in a newly deposited layer can be specified in the fields and in the values list in the `deposit` command, that is:

```
deposit PolySilicon type= isotropic rate= 1.0 time= 0.1 \
fields= {GSize Arsenic} values= {4e-6 1e19}
```

This will initialize the `GSize` to 40 nm and the arsenic concentration to a constant value of  $10^{19} \text{ cm}^{-3}$ . The `ArsenicGbc` solution will be created and the value of the corresponding dataset will be set automatically.

## Diffusion Equations

The diffusion in polycrystalline materials is modeled with two separate diffusion fluxes for the diffusion of  $C_A^+$  inside the grains and the diffusion of  $c_A^{gb}$  along the grain boundaries. The diffusion inside the grain regions is modeled as for crystalline silicon with the `ChargedFermi` diffusion model. The diffusion fluxes are scaled with the ratio of the grain boundary volume to the polysilicon volume, that is:

$$J_A = -f_g \sum_{X, c} D_{AX^c} \left( \frac{n}{n_i} \right)^{-c-z} \nabla \left( C_A^+ \left( \frac{n}{n_i} \right)^z \right) \quad (271)$$

$$\frac{\partial C_A}{\partial t} = -\nabla \bullet J_A - R \quad (272)$$

For details on the `ChargedFermi` model parameters, see [ChargedFermi Diffusion Model on page 188](#). The diffusivity  $D_{AX^c}$  for the grain interior is set as usual for the `ChargedFermi` model, for example:

```
pdbSet PolySilicon Boron Int Dstar \
{ 0 {[Arr 0.743e2 3.56]} 1 {[Arr 0.617e2 3.56]} }
```

## 4: Diffusion

### Diffusion in Polysilicon

For the fluxes along the grain boundaries, the gradient of the concentration in the grain boundary is multiplied by a constant diffusivity and the grain boundary volume share  $f_{gb}$ :

$$\frac{\partial C_A^{gb}}{\partial t} = -\nabla \bullet J_A^{gb} + R \quad (273)$$

$$J_A^{gb} = -f_{gb} D_A^{gb} \left( 1 - \frac{c_A^{gb}}{C_{Si}} \right) \nabla (c_A^{gb}) \quad (274)$$

The grain boundary diffusivity  $D_A^{gb}$  can be set in the parameter database using:

```
pdbSet PolySilicon Arsenic Dgb { [Arrhenius 1100.0 3.53] }
```

In polycrystalline materials, a segregation reaction is assumed to occur at the surface of the grains. The reaction describes the exchange of dopants between grain and grain boundary regions. The reaction term  $R$  is given as:

$$R = a(L) \cdot K \cdot \left[ C_A^+ \cdot \left( 1 - \frac{c_A^{gb}}{C_{Si}} \right) - \frac{c_A^{gb}}{s_g} \cdot \left( 1 - \frac{C_A^+}{C_{Si}} \right) \right] \quad (275)$$

The segregation term depends on the transport coefficient  $K$ , multiplied by the grain surface area per unit volume of polysilicon  $a(L)$ .

The transport coefficient  $K$  can be specified in the parameter database using:

```
pdbSet PolySilicon Arsenic Ksgb { [Arrhenius 1.630e4 3.586] }
```

The dopant segregation coefficient  $s_g$  for the segregation between the grain and grain boundary can be specified by using:

```
pdbSet PolySilicon Arsenic Sgb { [Arrhenius 2.75 -0.44] }
```

The grain surface area per unit volume  $a(L)$  depends on the grain structure. For columnar grain structures, this is:

$$a(L) = \frac{4 \cdot L}{(L + \delta)^2} \quad (276)$$

and, for cubic grains, this is:

$$a(L) = \frac{6 \cdot L^2}{(L + \delta)^3} \quad (277)$$

Table 15 Solution names

Symbol	Boron	Arsenic	Phosphorus	Antimony	Indium
$C_A$	Boron	Arsenic	Phosphorus	Antimony	Indium
$c_A^{gb}$	BoronGbc	ArsenicGbc	PhosphorusGbc	AntimonyGbc	IndiumGbc
$C_A^+$	BActive	AsActive	PActive	SbActive	InActive

Table 16 Solution names for granular model

Symbol	Solution name
$L$	GSize

## Anisotropic Diffusion Model

The behavior of dopants in polycrystalline materials is strongly influenced by the boundaries between crystalline grains. Dopant atoms tend to segregate from the interior of a grain to the boundaries, which provide paths for rapid diffusion. The rate of segregation depends on the rate of grain growth, while the number of diffusion paths along the boundaries depends on the grain size. In addition, the boundaries of the polycrystalline material act like grain boundaries, providing sites for electrically inactive dopant atoms and paths for diffusion. The diffusion equations for the grain-interior and grain-boundary components of the doping profile are solved separately. The equations are coupled by terms describing the segregation between the grain interiors and grain boundaries. To determine the rate of segregation and the density of grain-boundary diffusion paths, you also solve for the growth in grain size during high-temperature processing. The boundaries of the polycrystalline region are included as explicit grain boundaries in the diffusion and segregation equations. The model has been implemented in Sentaurus Process [7][8][9][10].

The model is invoked by specifying the polycrystalline material, for example:

```
pdbSet PolySilicon PolyCrystalline 1
```

To set the model to the TSUPREM-4 compatible mode, use the command:

```
SetTS4PolyMode
```

### Diffusion in Grain Interiors

Redistribution of dopants in polycrystalline materials occurs by the parallel diffusion of dopants through the interiors of grains and along grain boundaries.

## 4: Diffusion

### Diffusion in Polysilicon

In the grain interiors, diffusion of the active dopant is given by:

$$\frac{\partial c_g}{\partial t} = -\vec{\nabla} \cdot \left[ -D_g \left( \vec{\nabla} c_g - z_s c_g q \frac{\vec{E}_g}{kT} \right) \right] - G \quad (278)$$

where:

- $c_g$  is the active concentration in the grain interior.
- The diffusivity  $D_g$  and the electric field  $\vec{E}_g$  in the grain interior are calculated from the electron concentration  $n_g$ , which is in turn calculated from the doping concentrations  $c_g$ .
- $G$  accounts for the segregation of dopant to grain boundaries as described in [Segregation Between Grain Interior and Boundaries on page 232](#).

The parameter `Grain.Crystallinity` specifies the initial crystallinity of the grain interiors. If `Grain.Crystallinity` is set to `Crystalline`, the initial active concentration is determined by the `pdb` parameter `AcInit` or the term  `${Sol}AcInit`. If `Grain.Crystallinity` is set to `Amorphous`, the initial active concentration is determined by the `pdb` parameter `AmInit` or the term  `${Sol}AmInit`. The initialization is performed for the remainder after some implantation atoms go to a grain boundary according to [Eq. 287, p. 232](#).

## Grain Boundary Structure

Diffusion along grain boundaries is described in terms of the dopant concentration *per unit area* of grain boundary  $c_{gb}$ , and the average area of grain boundaries per unit volume:

$$\rho' = \rho + \delta_{if} \quad (279)$$

where  $\rho$  is the average area of grain boundaries per unit volume in the bulk of the poly layer and  $\delta_{if}$  accounts for the dopant at interfaces between poly and other materials (or ambient).  $\rho$  is inversely proportional to the average grain size  $L_g$ :

$$\rho = \frac{\text{GBGeomFactor}}{L_g} \quad (280)$$

where `GBGeomFactor` is a geometric factor specified for the polycrystalline material, for example:

```
 pdbSet PolySilicon GBGeomFactor 2.0
```

$\delta_{if}$  is a function of position defined by the fact that its integral over any volume is equal to the area  $A_{if}$  of the polysilicon interface passing through that volume:

$$\int \delta_{if} dV = A_{if} \quad (281)$$

The concentration of dopants in the grain boundaries per unit volume of material is then given by:

$$c_A^{gb} = \rho' c_{gb} \quad (282)$$

## Diffusion Along Grain Boundaries

The diffusion of dopant in the grain boundaries is given by:

$$\frac{\partial c_A^{gb}}{\partial t} = -\vec{\nabla} \cdot \left[ -FD_{gb} \left( \vec{\nabla} c_{gb} - z_s c_{gb} \frac{\vec{E}_{gb}}{kT} \right) \right] + G \quad (283)$$

The diffusivity  $D_{gb}$  and electric field  $\vec{E}_{gb}$  along the grain boundaries are calculated from the electron concentration  $n_{gb}$ ;  $n_{gb}$  is calculated by assuming that the net donor and acceptor concentrations are calculated from  $c_{gb}/K$ , the equilibrium dopant concentrations in the grain interior near the grain boundary, where  $K$  is the segregation coefficient given by [Eq. 289](#), [p. 232](#).  $G$  accounts for the segregation of dopant to grain boundaries as described in [Segregation Between Grain Interior and Boundaries on page 232](#).

Diffusivity  $D_{gb}$  is given by:

$$D_{gb} = Dgb \cdot \sum Dgb.Fermi \cdot \left( \frac{n_{gb}}{n_i} \right)^{-c} \quad (284)$$

$Dgb$  and  $Dgb.Fermi$  are defined by:

```
pdbSet <material> <dopant> Dgb <value>
pdbSet <material> <dopant> Dgb.Fermi <array>
```

$F$  is a tensor that describes the diffusion paths available to dopant in the grain boundaries. It is composed of two parts:  $F = F_b + (1 - F_{bu})F_{if}$ .  $F_b$  describes the available paths within the bulk of the poly layer. For a horizontal poly layer, it is given by:

$$F_b = \text{diag}\left(\frac{Dgb.F22}{L_g}, \frac{Dgb.F11}{L_g}, \frac{Dgb.F11}{L_g}\right) \quad (285)$$

Because of the columnar grain structure,  $Dgb.F22$  is larger than  $Dgb.F11$ , which implies that diffusion through the layer is faster than diffusion parallel to the layer.

$Dgb.F11$  and  $Dgb.F22$  are defined for the polycrystalline material, for example:

```
pdbSet PolySilicon Dgb.F11 1.0
pdbSet PolySilicon Dgb.F22 2.0
```

## 4: Diffusion

### Diffusion in Polysilicon

$F_{if}$  describes the available paths for diffusion along material interfaces. In the vicinity of a horizontal interface, it has the value:

$$F_{if} = \text{diag}(0, \delta_{if}, \delta_{if}) \quad (286)$$

For the interface between polysilicon and silicon, the phenomenon of interfacial breakup accompanied by epitaxial realignment can occur, as described in [Interface Oxide Breakup and Epitaxial Regrowth on page 236](#).  $F_{bu}$  is the fraction of the polysilicon–silicon interface that has broken up. For layers or interfaces that are not horizontal,  $F_b$  and  $F_{if}$  are rotated by the angle of the layer or interface, respectively, with respect to the horizontal axis.

## Segregation Between Grain Interior and Boundaries

When dopant is initially introduced into a polycrystalline material, some of the dopant occupies sites in the interior of a grain and some occupies sites on a grain boundary. The initial segregation of dopant is given by:

$$c_{gb} = \frac{\text{GBMaxDensity}}{\text{GMaxConc}} \text{GSegInit } c_g \quad (287)$$

`GBMaxDensity`, `GMaxConc`, and `GSegInit` represent the density of available sites on grain boundaries, and in the grain interiors and the initial segregation entropy, respectively. In the case of ion implantation,  $c_g$  and  $c_{gb}$  describe the additional dopant introduced by the implantation; dopant that is present before the implantation is not redistributed.

Dopant atoms are free to move between sites in the interior of a grain and sites on the grain boundary during high-temperature processing. The rate of segregation is given by:

$$G = (\rho q_b + (1 - F_{bu})\delta_{if}q_{if}) \left( f_{gb} c_g - f_g \frac{c_{gb}}{K} \right) \quad (288)$$

The segregation coefficient  $K$  is given by [11]:

$$K = \frac{\text{GBMaxDensity}}{\text{GMaxConc}} \text{Sgb} \quad (289)$$

`GBMaxDensity`, `GMaxConc`, `GSegInit`, and `Sgb` are defined for dopants, for example:

```
pdbSet PolySilicon Dopant GBMaxDensity 2.5e15
pdbSet PolySilicon Dopant GMaxConc 5e22
pdbSet PolySilicon Dopant GSegInit 1.0
pdbSet PolySilicon Boron Sgb { [Arrhenius 0.2 -0.38] }
```

The segregation velocities associated with the bulk of the poly region and the material interfaces are given by:

$$q_b = \frac{1}{GBVFactor} \frac{\partial L_g}{\partial t} + KsgbFactor \frac{D_g}{L_g} \quad (290)$$

`GBVFactor` is the parameter for the material. `KsgbFactor` and  $q_{if}$ , which is defined by `Vsgb`, are specified for dopants. For example:

```
pdbSet PolySilicon GBVFactor 1.33
pdbSet PolySilicon Dopant KsgbFactor {[Arr 4.0 0.0]}
pdbSet PolySilicon Dopant Vsgb {[Arr 1e7 3.0]}
```

$f_g$  and  $f_{gb}$  are the fractions of unfilled interior and boundary sites:

$$f_g = 1 - \frac{c_g}{GMaxConc} \quad (291)$$

$$f_{gb} = 1 - \sum \frac{c_{gb}}{GBMaxDensity} \quad (292)$$

where the sum is taken over all the dopant species present in the structure.  $F_{bu}$  is the fraction of the polysilicon–silicon interface that has broken up, as described in [Interface Oxide Breakup and Epitaxial Regrowth on page 236](#).

## Grain Size Model

The grains in the polycrystalline material are assumed to be oriented as columns that extend through the wafer. The structure is characterized by  $L_g$ , the average grain size in the lateral direction (in other words, in the plane of the layer), and a vector describing the orientation of the columnar grains.

The initial grain size is determined by the temperature of the poly deposition process:

$$L_g = \begin{cases} \max(\text{Frac.TA} \times t_a, \text{GrainSize}) & T_c \leq \text{GrainSizeTempC} \\ \text{GrainSize} + 2 \cdot \text{GrainSizeFactor} \cdot z & T_c > \text{GrainSizeTempC} \end{cases} \quad (293)$$

where:

- $T_c$  is the deposition temperature (specified in the `deposit` command) in degree Celsius.
- $t_a$  is the thickness of the amorphous silicon layer produced by low-temperature deposition.
- $z$  is the distance from the bottom of the layer.

For high-temperature depositions, grain size depends on the thickness specified in the `deposit` command. Dividing a deposition into multiple smaller depositions produces

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### Diffusion in Polysilicon

different results for the grain size. For low-temperature depositions, the material is assumed to be amorphous (a negative grain size is reported in printing or plotting). The initial grain size is calculated from the thickness  $t_a$  of the amorphous layer at the beginning of the next diffusion step.

`Frac.TA`, `GrainSize`, `GrainSizeFactor`, and `GrainSizeTempC` are the material parameters, for example:

```
pdbSet PolySilicon Frac.TA 0.5
pdbSet PolySilicon GrainSize 5e-6 ;# cm
pdbSet PolySilicon GrainSizeFactor {[Arr 0.1 0.0]}
pdbSet PolySilicon GrainSizeTempC 600.0
```

## Surface Nucleation Model

An alternative model for the standard grain size model (see [Grain Size Model on page 233](#)) is the surface nucleation model. In this model, grains are assumed to grow from small clusters formed at the early stages of deposition. The kinetics of nucleation, under this assumption, determines the average distance between clusters, thereby, the average starting grain size near the surface upon which deposition occurs. The model for atomistic nucleation is derived from rate equations for growth, surface diffusion, and desorption [\[12\]](#). Different regimes are considered:

- Large deposition rates (compared to surface diffusion or evaporation) are labeled *complete condensation*.
- Conditions where the deposition rate between surface diffusion and evaporation are labeled *incomplete condensation*.
- Low deposition rates are labeled *extremely incomplete condensation*.

Besides the deposition rates, two types of nuclei are considered: 2D or 3D islands. The following formula computes the nucleation density:

$$n = n_0 R^p \exp\left(\frac{E}{kT}\right) \quad (294)$$

where  $p$  and  $E$  are given by [Table 17 on page 235](#). The choice of regime is set with:

```
pdbSet SNG.Model <regime>
```

where `<regime>` is one of `Complete`, `Initially.Incomplete`, `Extreme.Incomplete`, or `None` (default) meaning the model is switched off.

Table 17 Formulas for surface nucleation model

Regime	3D islands	2D islands
Extremely incomplete	$p = \frac{2}{3}i$ $E = \frac{2}{3}(E_i + (i+1)E_a - E_d))$	$p = i$ $E = E_i + (i+1)E_a - E_d)$
Incomplete	$p = \frac{2}{5}i$ $E = \frac{2}{5}(E_i + iE_a)$	$p = \frac{i}{2}$ $E = E_i + iE_a$
Complete	$p = i/(i+2.5)$ $E = (E_i + iE_d)/(i+2.5)$	$p = i/(i+2)$ $E = (E_i + iE_d)/(i+2)$

**NOTE** Default values for parameters of the surface nucleation model have not been calibrated for any process. They have simply been set to give approximately the same values as the grain size model in polysilicon diffusion.

Table 18 Parameters of surface nucleation model set with  
pdbSet PolySilicon <parameter> <value>

Symbol	Parameter name
Island dimension	SNG.Island.Dim
$R$	SNG.Growth.Flux
$n_0$	SNG.Prefactor
$i$	SNG.Critical.Island.Size
$E_a$	SNG.Adsorption.Energy
$E_d$	SNG.Diffusion.Energy
$E_i$	SNG.Critical.Island.Energy

## Grain Growth

The growth of the grains during high-temperature processing is given by [13]:

$$\frac{\partial L_g}{\partial t} = \frac{1}{L_g} A0 \times DselfFactor \times Dself \times \frac{E_{gb}}{kT} \times F_{seg} + G_{EA} \quad (295)$$

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### Diffusion in Polysilicon

$A_0$ ,  $D_{selfFactor}$ , and  $D_{self}$  represent the empirical geometric factor, the enhancement factor of silicon self-diffusivity at the grain boundary, and the silicon self-diffusivity in the vicinity of a grain boundary, respectively:

```
pdbSet PolySilicon A0 6.0
pdbSet PolySilicon DselfFactor { [Arrhenius 5.6e-6 -1.73] }
pdbSet PolySilicon Dself { -2 { [Arrhenius 5.6e-6 2.86] }
                           -1 0.0
                           0 { [Arrhenius 4.29e-7 2.18] }
                           1 0.0
                           2 0.0 }
```

$E_{gb}$  is the surface energy per atom associated with the grain boundary [13][14][15];  $F_{seg}$  models the segregation drag effect; and  $G_{EA}$  models epitaxial regrowth of the poly layer (see [Interface Oxide Breakup and Epitaxial Regrowth on page 236](#)).

$$E_{gb} = (2 \cdot \text{LatticeSpacing} \cdot \text{Tu})^2 \cdot \text{Lambda} \cdot \left( \frac{1}{1 + \text{Lambda} \cdot hf_n} + \text{Lambda} \cdot 1 \frac{L_g}{t_{poly}} \right) \quad (296)$$

$$f_n = \begin{cases} \frac{L_g}{2t_{poly} - L_g} & L_g < t_{poly} \\ \frac{L_g}{t_{poly}} & L_g \geq t_{poly} \end{cases} \quad (297)$$

$t_{poly}$  is the thickness of the polycrystalline layer.

The segregation drag effect reduces the grain growth rate [16]:

$$F_{seg} = \left( 1 + \sum \frac{c_{gb}}{\text{GBMaxDensity}} \right)^{-\text{SegDragExponent}} \quad (298)$$

`SegDragExponent` is defined for the material, for example:

```
pdbSet PolySilicon SegDragExponent 2.0
```

## Interface Oxide Breakup and Epitaxial Regrowth

A thin interfacial oxide layer is typically present between a deposited polysilicon layer and any underlying single-crystal silicon. This interfacial oxide presents a barrier to epitaxial realignment of the poly layer. With sufficient high-temperature processing, the oxide layer breaks up into a discrete set of small spheres, allowing epitaxial regrowth of the poly to proceed.

The oxide breakup is modeled by the formation of voids in the interfacial oxide layer [17]–[20]. The radius of the voids  $R_{void}$  increases as:

$$\frac{dR_{void}}{dt} = \frac{\beta}{t_{ox}^3} \times \exp\left(-\frac{E_{bu}}{kT}\right) \quad (299)$$

where:

- $\beta$  is a constant.
- $t_{ox}$  is the initial oxide thickness.
- $E_{bu}$  is the activation energy of the breakup process.
- $R_{void}$  is initialized to zero whenever poly is deposited on exposed silicon.

The fraction of the interface that is broken up is given by:

$$F_{bu} = 1 - \exp(-\pi N_{EA} R_{void}^2) \quad (300)$$

where  $N_{EA}$  is the areal density of the voids.

The parameters for the model are specified in terms of a characteristic breakup time for the thinnest (5 Å) interfacial oxide layers:

$$t_{bu} \equiv \frac{5\dot{A}^3}{\sqrt{\pi N_{EA}} \beta} \times \exp\left(\frac{E_{bu}}{kT}\right) \quad (301)$$

$t_{bu}$  is defined with the parameter PolyOxBreakTime, for example:

```
pdbSet PolySilicon PolyOxBreakTime { [Arrhenius 1.0 -5.0] } ;# seconds
```

$$\frac{dR_{void}}{dt} = \frac{1}{t_{bu}} \left( \frac{5\dot{A}}{t_{ox}} \right)^3 \frac{1}{\sqrt{\pi N_{EA}}} \quad (302)$$

In the present implementation, assume that all polycrystalline or single-crystalline interfaces share a common oxide thickness given by:

$$t_{ox} = \text{PolyOxThickness} \quad (303)$$

PolyOxThickness is defined in the material:

```
pdbSet PolySilicon PolyOxThickness 5e-8 ;# cm
```

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### Diffusion in Polysilicon

Epitaxial regrowth is modeled by increasing the poly grain size to a value larger than the thickness of the poly layer. This grain growth is described by  $G_{EA}$  in Eq. 286, p. 232 for the grain size:

$$G_{EA} = F_{bu} v_{EA} \delta_{if} \quad (304)$$

It serves as a driving force for epitaxial regrowth from the interface at the silicon–polysilicon interface. Parameters for this model are given by:

$$v_{EA} = \text{EpiGrowthVelocity} \quad (305)$$

```
pdbSet PolySilicon EpiGrowthVelocity {[Arrhenius 100.0 3.0]} ;# cm2/s
```

## Dependence of Polysilicon Oxidation Rate on Grain Size

It has been observed experimentally that the oxidation rate for fine-grained polysilicon is faster than for coarser-grained polycrystalline or single-crystalline silicon, presumably because of enhanced oxidation at the grain boundaries.

You can model this enhancement by assuming a faster surface reaction rate where grain boundaries intersect the oxide–poly interface:

$$k_s = (1-f)k_g + fk_{gb} \quad (306)$$

where:

- $k_g = \frac{BC_{ox}}{AC^*}$  is the surface reaction rate in the absence of grain boundaries.
- $k_{gb}$  is the reaction rate at a grain boundary.
- $f = \min\left(\frac{\delta T}{L_g}, 1\right)$  is the fraction of the surface within a distance  $\delta T/2$  of a grain boundary.

The enhancement factor at grain boundaries is specified as:

$$\frac{k_{gb}}{k_g} = \text{GBFactor} \quad (307)$$

```
pdbSet Oxide_PolySilicon H2O GBFactor {[Arr 10.0 0.0]}  
pdbSet Oxide_PolySilicon O2 GBFactor {[Arr 10.0 0.0]}  
pdbSet Oxide_PolySilicon N2O GBFactor {[Arr 10.0 0.0]}
```

The effective thickness of the grain boundaries is given by  $\delta T = \text{GBEffThick}$ , where  $\text{GBEffThick}$  is specified for each material.

## Boundary Conditions

### Boundary Conditions for Grain Growth Equation

Several boundary conditions are available to control the grain size (`GSize`) in the grain growth equation. The reflective (`HomNeumann`) boundary condition assumes that the interface value grows like the bulk value. The minimum value (`MinimumSize`) boundary condition sets the interface value at the minimum value for `GSize`. The minimum value is set with:

```
pdbSet <material> GSize minConc {<n>}
```

The initial size (`InitialSize`) boundary condition fixes the interface value at the initial value of `GSize`.

The boundary conditions can be switched on using:

```
pdbSet Oxide_PolySilicon GSize BoundaryCondition  
[{HomNeumann MinimumSize InitialSize}]
```

The default setting for the grain growth boundary condition is `HomNeumann`.

### Dopant Diffusion Boundary Conditions

There are three additional segregation-type boundary conditions available with the polycrystalline diffusion model. The first can be selected with:

```
pdbSet Oxide_PolySilicon Arsenic BoundaryCondition GrainBoundarySegregation
```

The total dopant fluxes at the interfaces between the grain boundary and the neighboring layer are balanced. The fluxes are given by:

$$\mathbf{j} \bullet \mathbf{n} = k_{Transfer} \left( C_A^{other} - \frac{C_A^{gb}}{f_{gb} s_g k_{Segregation}^{gb}} \right) \quad (308)$$

where  $C_A^{other}$  is the concentration of dopant on the other side of the interface,  $C_A^{gb}$  is the grain boundary concentration,  $k_{Transfer}$  is the transfer rate, and  $k_{Segregation}^{gb}$  is the segregation rate of dopant A in the grain boundary.

To set these parameters, use:

```
pdbSet <interface_material> <dopant> Transfer {<n>}  
pdbSet <interface_material> <dopant> SegregationGb {<n>}
```

The coefficient  $s_g$  is the grain-grain boundary segregation coefficient.

## 4: Diffusion

### Diffusion in Polysilicon

To select the second boundary condition, use:

```
pdbSet Oxide_PolySilicon Arsenic BoundaryCondition  
    GrainGrainBoundarySegregation
```

The total dopant fluxes at the interfaces between the grain and the neighboring layer and the grain boundary and neighboring layer are balanced. The fluxes are given by:

$$\mathbf{j}_g \bullet \mathbf{n} = k_{Transfer} \left( C_A^{other} - \frac{f_g C_A^+}{k_{Segregation}} \right) \quad (309)$$

$$\mathbf{j}_{gb} \bullet \mathbf{n} = k_{Transfer} \left( C_A^{other} - \frac{C_A^{gb}}{s_g k_{Segregation}^{gb}} \right) \quad (310)$$

and:

$$\mathbf{j} \bullet \mathbf{n} = \mathbf{j}_g \bullet \mathbf{n} + \mathbf{j}_{gb} \bullet \mathbf{n} \quad (311)$$

where  $C_A^+$  is the active concentration of dopant in the grain and  $k_{Segregation}$  is the segregation rate of dopant A in the grain. To set this parameter, use:

```
pdbSet <interface material> <dopant> Segregation {<n>}
```

To select the third boundary condition, use:

```
pdbSet Oxide_PolySilicon Arsenic BoundaryCondition \  
    BulkGrainBoundarySegregation
```

The total dopant fluxes at the interfaces between the grain and the neighboring layer and between the grain and the grain boundary are balanced. The fluxes are given by:

$$\mathbf{j} \bullet \mathbf{n} = k_{Transfer} \left( C_A^{other} - \frac{f_g C_A^+}{k_{Segregation}} \right) \quad (312)$$

$$\mathbf{j}_{gb} \bullet \mathbf{n} = k_{Transfer} \left( \frac{f_g C_A^+}{k_{Segregation}} - \frac{C_A^{gb}}{f_{gb} s_g k_{Segregation}^{gb}} \right) \quad (313)$$

**NOTE** For the anisotropic polycrystalline model, use the Segregation model for the boundary condition:

```
pdbSet PolySilicon_Silicon Boron BoundaryCondition Segregation  
pdbSet Oxide_PolySilicon Boron BoundaryCondition Segregation  
pdbSet Gas_PolySilicon Boron BoundaryCondition Segregation
```

## Dopant Diffusion in Silicon Germanium

The presence of germanium in silicon affects dopant diffusion in various ways. The Constant diffusion model and the Interdiffusion model are available for germanium diffusion in silicon (see [Constant Diffusion Model on page 191](#) and [SiGe Interdiffusion Model](#)). By default, the Constant diffusion model is set for germanium diffusion in silicon (and for silicon diffusion in germanium).

Germanium is defined as a silicon-like material and has the same terms of silicon if the terms are not defined otherwise.

---

## SiGe Interdiffusion Model

Defect-mediated interdiffusion of silicon and germanium can be set using the following switches:

```
pdbSet Silicon Germanium DiffModel Interdiffusion
pdbSet Germanium Silicon DiffModel Interdiffusion
```

**NOTE** These switches are set automatically when using Advanced Calibration together with `Ge_Chem_Eff 1` in the `SiGe_and_Stress_Effect` procedure to switch on the recommended models and parameters in SiGe (see [Advanced Calibration for Process Simulation User Guide, Ge Chemical Effect \(Ge\\_Chem\\_Eff\) on page 39](#)).

In SiGe, the interdiffusion of Si and Ge atoms is a consequence of point-defect diffusion [21]. Contributions from a direct exchange mechanism can be neglected. SiGe interdiffusion is described as the sum of a contribution from vacancy diffusion and a contribution from interstitial diffusion [22]. Therefore, interdiffusion in SiGe can be described by the following equations:

$$\frac{d}{dt}C_{\text{Ge, Si}} = \nabla \bullet (D_{\text{inter}} \nabla C_{\text{Ge, Si}}) - \nabla \bullet \left( D_{\text{inter}} C_{\text{Ge, Si}} \cdot (1 - \text{xMoleFraction}) \frac{\Delta V}{k_B T} \nabla P \right) \quad (314)$$

$$D_{\text{inter}} = D_{\text{inter}}^V D_{\text{VF}} \frac{C_V}{C_{\text{V(intrinsic)}}^*} D_{\text{interF}}^V + D_{\text{inter}}^I D_{\text{IF}} \frac{C_I}{C_{\text{I(intrinsic)}}^*} D_{\text{interF}}^I \quad (315)$$

where:

- $C_{\text{Ge}}$  (or  $C_{\text{Si}}$ ) are concentrations of Ge (or Si) atoms in SiGe material based on Silicon (or Germanium) material, respectively. Since the sum of Si and Ge atoms is given by the lattice density, it is sufficient to solve only one equation for  $C_{\text{Ge}}$  or  $C_{\text{Si}}$ . For most

## 4: Diffusion

### Dopant Diffusion in Silicon Germanium

applications, SiGe is considered to be silicon with Ge as an impurity, in which case, [Eq. 314](#) must be solved for  $C_{\text{Ge}}$  only.

- $k_B$  is the Boltzmann constant, and  $T$  is the temperature in kelvin.
- $\Delta V$  is a parameter with the dimension of volume.
- $P$  is the pressure.

[Eq. 315](#) computes the integral coefficient of interdiffusion  $D_{\text{inter}}$ . It consists of interstitial and vacancy components.  $C_V$  and  $C_I$  are the concentrations of vacancies and interstitials, respectively.  $D_{\text{inter}}^V$  and  $D_{\text{inter}}^I$  are the interdiffusion coefficients in undoped and unstrained SiGe for the vacancy and interstitial mechanisms, respectively. They are Ge mole fraction-dependent parameters and can be set using the PDB parameter `D.Inter` in the materials Silicon and Germanium for Interstitial and Vacancy defects:

```
pdbSet Silicon Int D.Inter {[Arr 1400 4.95]}\n pdbSet Germanium Int D.Inter {[Arr 353 4.28]}\n pdbSet Silicon Vac D.Inter {[ArrBreak 240 4.69 2343.304 4.94 1000]}\n pdbSet Germanium Vac D.Inter {[Arr 41.6 3.32]}
```

By default, the following coefficients are used for quadratic interpolation of `D.Inter` parameters:

```
pdbSet SiGe Int D.Inter.X2 {[Arr 0.0016 -0.29]}\n pdbSet SiGe Vac D.Inter.X2 {[Arr 2.6e5 1.52]}
```

The quantities  $C_{V(\text{intrinsic})}^*$  and  $C_{I(\text{intrinsic})}^*$  are the equilibrium concentrations of the vacancies and interstitials in the intrinsic material. By default, they follow an Arrhenius law and can be changed using the command:

```
pdbSet <material> <defect> Cstar {<n>}
```

The following factors are necessary to include effects of doping and mechanical strain in SiGe. They are defined as terms (see [Effect of Germanium on Point-Defect Parameters on page 248](#)), which are equal to 1.0 if not redefined by other Sentaurus Process models or by users. The contribution from vacancy diffusion is multiplied by all of the following factors:

- $D_{VF}$  is `VacDiffFactor`. It takes into account that the diffusivity of vacancies is modified in strained SiGe, as a function of pressure.
- $D_{\text{interF}}^V$  is `InterVDiffFactor`. It has a constant value 1.0 by default and serves as a placeholder for users who want to include contributions from dopant–vacancy pair diffusion to SiGe interdiffusion. For SiGe with a high concentration of As or P, it is possible that a significant or even dominant contribution to the intermixing of Si and Ge atoms is caused by As–V or P–V pair diffusion not present in undoped SiGe.

Similarly, the contribution to SiGe interdiffusion from interstitial diffusion contains the corresponding factors:

- $D_{IF}$  is IntDiffFactor.
- $D_{interF}^I$  is InterIDiffFactor.

The second term in Eq. 314 corresponds to the Ge (or Si) atoms flux contribution, which is proportional to the gradient of P (pressure). Therefore, it can be called the *interdiffusion drift term*. Usually, it is smaller than the flux in the first term, which is proportional to the gradient of  $C_{Ge}$  (or  $C_{Si}$ ).

The interdiffusion drift term is switched off by default and is switched on by the following parameters:

```
pdbSet Silicon Germanium Interdiffusion.Drift 1
pdbSet Germanium Silicon Interdiffusion.Drift 1
```

The  $\Delta V$  parameter corresponds to the difference of atomic volumes between the two basic materials. It does not depend on the Ge mole fraction in SiGe and has the dimension  $10 \cdot m^3 \cdot eV/J$ . It is defined by the following parameters in materials Silicon and Germanium, respectively:

```
pdbSet Silicon Germanium Interdiffusion.Drift.Vol 1.65e-12
pdbSet Germanium Silicon Interdiffusion.Drift.Vol -1.65e-12
```

## Low-to-High Germanium-Doped SiGe Model

The diffusion model in SiGe described in [Low Germanium-Doped SiGe Model on page 245](#) is based on a silicon material-oriented approach by fine-tuning the parameters (using either the term command or a specific procedure) of silicon material. However, this approach is only applicable for low Ge mole fraction. For high mole-fraction Ge, such an approach does not work. Even when you have adjusted for Ge-doped Si and Si-doped Ge, it is not guaranteed that both will give the same (at least similar) results for near 0.5 mole-fraction cases, which requires the correct application window.

The low-to-high Ge-doped SiGe model uses the values of physical PDB parameters depending on the Ge concentration, which are interpolated with those for silicon and germanium materials. The model provides the solution to apply all ranges of mole fraction ( $0 \leq x \leq 1$  ).

The parameter interpolation is switched on using:

```
pdbSet Diffuse Parameter.Interpolation 1 ;# default=1
```

## 4: Diffusion

### Dopant Diffusion in Silicon Germanium

The model is applied to a Ge-doped silicon material if the maximum Ge concentration in the silicon region exceeds Min.Conv.Conc and the Skip.Parameter.Interpolation parameter is switched off as follows:

```
pdbSet SiGe Ge Min.Conv.Conc 5E20          ;# default=5E20
pdbSet Silicon Skip.Parameter.Interpolation 0 ;# default=1
```

Likewise, for a Si-doped germanium material:

```
pdbSet SiGe Si Min.Conv.Conc 5E20          ;# default=5E20
pdbSet Germanium Skip.Parameter.Interpolation 0 ;# default=1
```

For SiGe material, the model is switched on by default. To switch it off, use:

```
pdbSet SiGe Skip.Parameter.Interpolation 1      ;#default=0
```

For details, see [Alloy Materials and Parameter Interpolation on page 25](#).

## Defining Mole Fractions

At the beginning of diffusion, the xMoleFraction term is defined with the lattice density of silicon ( $LD_{Si}$ ) and germanium ( $LD_{Ge}$ ) as follows:

- For Ge-doped silicon material:

$$xMoleFraction = 2 \frac{C_{Ge}}{LD_{Si} + \sqrt{LD_{Si}^2 + 4C_{Ge}(LD_{Ge} - LD_{Si})}} \quad (316)$$

- For Si-doped germanium material:

$$xMoleFraction = 1 - 2 \frac{C_{Si}}{LD_{Ge} + \sqrt{LD_{Ge}^2 + 4C_{Si}(LD_{Si} - LD_{Ge})}} \quad (317)$$

- For Si-doped or Ge-doped SiGe material:

$$xMoleFraction = \frac{C_{Ge}}{C_{Ge} + C_{Si}} \quad (318)$$

where the silicon concentration is calculated by solving:

$$\frac{\partial C_{Si}}{\partial t} = -\frac{2(C_{Ge} + C_{Si}) - LD_{Ge}}{2(C_{Ge} + C_{Si}) - LD_{Si}} \frac{\partial C_{Ge}}{\partial t} \quad (319)$$

## Bandgap Model

The change in the energy bandgap along with the mole fraction shows a very nonlinear curve due to the transition between the X-valley ( $x < 0.8$ ) and the L-valley ( $x > 0.8$ ). To model such nonlinearity, the parameter `de1Eg.Function` for the interpolation method is set in SiGe material. The function returns the string expression fed to the potential equation:

$$\Delta E_g = (0.3758(0.7795 - x)^2 - 0.22835) - 0.2406 \exp\left(-\left(\frac{1-x}{0.1176}\right)^2\right) \quad (320)$$

**NOTE** The following models are not supported yet for the low-to-high Ge-doped SiGe model:

- Other defect clustering model than 1Moment
- EOR dopant trapping model
- BIC
- N<sub>2</sub> dimer model

**NOTE** If a Ge–Si (doped with respective alloy) interface is present, for example, Si-doped germanium deposited on silicon, the boundary condition at the Ge–Si interface should be Continuous.

## Low Germanium-Doped SiGe Model

First, the band gap of silicon is lowered in the presence of germanium. Second, germanium affects the point-defect equilibrium concentration. In addition, germanium can pair with boron forming an immobile but electrically active species.

### Bandgap Effect

The effect of bandgap narrowing on the dopant diffusion arises from the change in the intrinsic carrier concentration  $n_i(Si)$ . This has been implemented in Sentaurus Process as follows:

$$n_i = n_i(Si) e^{\frac{-\Delta E_g}{2kT}} \quad (321)$$

where  $\Delta E_g$  is bandgap narrowing due to germanium content. It can be defined using the command:

```
pdbSet <material> Germanium de1Eg {<n>}
```

## 4: Diffusion

### Dopant Diffusion in Silicon Germanium

The band gap, `de1Eg` ( $\Delta E_g$ ), is a function of germanium concentration and is given by:

$$\Delta E_g \equiv \Delta E_{gs} + (\Delta E_{gr} - \Delta E_{gs})(1 - Fpm) \quad (322)$$

$$\Delta E_{gs} = 0.835x^2 - 1.01x \quad (323)$$

$$\Delta E_{gr} = 0.33x^2 - 0.55x \quad (324)$$

$$x = \frac{C_{Ge}}{5.0 \times 10^{22}} \quad (325)$$

where  $\Delta E_{gs}$  [23] is the bandgap narrowing in strained silicon,  $\Delta E_{gr}$  [24] is the bandgap narrowing in the relaxed silicon,  $Fpm$  is a pseudomorphic factor that shows the degree of the relaxation, and  $x$  is the germanium fraction in silicon.  $Fpm$  is calculated with respect to lattice mismatch in the substrate. For example:

$$Fpm = \frac{(a_{SiGe} - a)}{a_{SiGe} - a_{Si}} \quad (326)$$

where:

- $a_{SiGe}$  is the lattice-spacing of the silicon-germanium region.
- $a_{Si}$  is the lattice-spacing of silicon.
- $a$  is the lattice-spacing calculated in the mechanics.

If the system is fully relaxed,  $Fpm$  is zero. If it is fully strained,  $Fpm$  is one.  $\Delta E_g$  will be used if the germanium percentage is greater than 0.1% (if parameter interpolation is not used and the default PDB parameter `<material> Germanium de1Eg { [Gede1Eg] }` is used together with the default procedure `Gede1Eg`), and the bandgap narrowing effects due to other strain sources will be ignored (see [Pressure-Dependent Defect Diffusion on page 259](#)).

## Potential Equation

The permittivity of ‘Ge-doped’ silicon can be calculated by the following formula, in which  $x_{Ge}$  is the germanium concentration in silicon:

$$\epsilon = (1 - x_{Ge}) \times \epsilon_{Si} + x_{Ge} \times \epsilon_{Ge} \quad (327)$$

where  $\epsilon_{Si}$  and  $\epsilon_{Ge}$  are defined as PDB parameters:

```
 pdbSet Ge Potential Permittivity 15.8  
 pdbSet Si Potential Permittivity 11.7
```

This calculation is included when setting:

```
pdbSetString Si CompSpecies "Germanium"
pdbSetBoolean Si Potential PermittivityContentEffect 1
```

The product of the density-of-states in the conduction and valence bands,  $N_c \times N_v$ , is multiplied by the factor defined as:

```
pdbSetFunction Si Ge factorNcNv [GefactorNcNv]
```

when the following PDB value is set:

```
pdbSetBoolean Si Potential BandgapContentEffect 1
```

Such a factor can be defined as:

$$(1 - x_{\text{Ge}} \times 0.47 / 0.81)^{3/4} \quad (328)$$

with the following line:

```
fproc GefactorNcNv { } { return "(1.0-(Germanium/5.0e22)*0.47/0.81)^0.75" }
```

## Effects on Point-Defect Equilibrium Concentrations

The introduction of germanium acts thermodynamically on the equilibrium of the silicon matrix. Compressive strain increases the equilibrium concentration of vacancies and decreases the equilibrium concentration of interstitials, and the tensile strain has the opposite effect on the point-defect equilibrium concentrations [25][26].

These effects are modeled in Sentaurus Process by modifying the equilibrium point-defect concentrations:

$$C_X^* = C_X^*(Si, P=0) e^{\frac{-(\Delta V_X P + \Delta V_{GeX})}{kT}} \quad (329)$$

$$\Delta V_{GeX} = \Delta V_{olGeX} \Delta a_{SiGe} \frac{C_{Ge}}{5 \times 10^{22}} \quad (330)$$

where  $C_X^*$  is the equilibrium concentration of point defects (interstitial or vacancy), and  $\Delta V_X$  is the activation volume change of equilibrium point defects due to the pressure  $P$ .

The following set of commands can be used to modify  $\Delta V_X$ :

```
pdbSet Silicon Interstitial Volume 8.59e-24
pdbSet Silicon Vacancy Volume -5.52e-24
```

## 4: Diffusion

### Dopant Diffusion in Silicon Germanium

To switch on strain effects on point defects, set the following switches:

```
pdbSet Silicon Interstitial CStarMod FermiPressureDependent  
pdbSet Silicon Vacancy CStarMod FermiPressureDependent
```

$\Delta V_{GeX}$  is the total activation volume change of equilibrium point defects due to the presence of germanium and is calculated from the activation volume change  $\Delta V_{olGeX}$ , the lattice mismatch coefficient  $\Delta a_{SiGe}$ , and the germanium fraction in the structure (see Eq. 330). These quantities can be modified using the following commands:

```
pdbSet Silicon Germanium Interstitial delVol 11.8  
pdbSet Silicon Germanium Vacancy delVol 25.6  
pdbSet Silicon Germanium LatticeMismatch 0.0425
```

**NOTE** The parameter `delVol` is given in units of eV, and `Volume` is given in units of  $\text{cm}^3$ .

## Effect of Germanium on Point-Defect Parameters

You can define arbitrary Alagator expressions for the point-defect basic parameter prefactors. The names of terms used for the vacancy and interstitial equilibrium concentration are `VacCStarFactor` and `IntCStarFactor`, respectively. Corresponding terms for the vacancy and interstitial diffusivity are `VacDiffFactor` and `IntDiffFactor`. These expressions can be used to include the effect of germanium on point-defect parameters. For example, the prefactor for the vacancy equilibrium concentration in SiGe can be calculated as follows:

```
MultiplyTerm Si VacCStarFactor "exp((1.088*($x_Ge))*$Vt_i)"
```

where `x_Ge` is the germanium content, and `vt_i` is  $1/(kT)$  in  $\text{eV}^{-1}$ .

**NOTE** By default, the `MultiplyTerm` command is not saved to TDR files. If the command file is split, this command must be included in the new command file. Alternatively, to save `MultiplyTerm` to TDR files, define `MultiplyTerm` with the keyword `store`.

## Impact of Germanium on Extended-Defect Parameters

The parameters `IClusterDissIntFactor`, `C311DiffIntFactor`, and `CLoopTransfer` (used in the `Full` model for I-clusters) can be used to include the impact of germanium on extended defects.

## Impact of Dopant Diffusivities

The germanium chemical effect is simulated by the activation energy correction using diffusivity prefactors. For example, in the case of boron, it is performed by the term `BoronIntDiffFactor`, which can be defined in silicon:

```
MultiplyTerm Si BoronIntDiffFactor "exp(-0.227*($x_Ge)*$Vt_i)"
```

**NOTE** By default, the `MultiplyTerm` command is not saved to TDR files. If the command file is split, this command must be included in the new command file. Alternatively, to save `MultiplyTerm` to TDR files, define `MultiplyTerm` with the keyword `store`.

During assembly of the diffusion equations, Sentaurus Process checks each dopant and material for whether such diffusion factors exist. The diffusivity through dopant–interstitial or dopant–vacancy pairs is then multiplied by the corresponding diffusion enhancement factors. A separation between interstitial and vacancy effects is necessary because with increasing germanium content of SiGe, the fractions of diffusion mediated by dopant–interstitial and dopant–vacancy pairs change.

## SiGe Strain and Dopant Activation

The solid solubility of dopants depends on the strain. In general, for compressive strain, the solubility of atoms smaller than silicon increases; whereas, the solubility of larger atoms decreases. In the Transient model, the stress effect is taken into account by introducing the pressure-dependent parameters `Solubility` and `TotalSolubility`:

$$S(P) = S(P = 0)\exp(-P V/kT) \quad (331)$$

An example of the definition of boron pressure-dependent solid solubility is:

```
pdbSet Si B SS.Factor "exp(3.636e-24*Pressure*$kT_i)"
pdbSet Si B Total.SS.Factor "exp(3.636e-24*Pressure*$kT_i)"
```

Since the emission rate for the silicon side in the three-phase segregation model is proportional to the solid solubility, a corresponding modification also must be included in the boundary condition. For example, this can be achieved by the following line for boron:

```
pdbSetString Si B Side.SS.Factor "exp(3.636e-24*Pressure_Silicon*$kT_i)"
```

**NOTE** You can define the arbitrary Alagator expressions for the dopant solid solubility prefactors in Sentaurus Process. The name of strings used for the solid solubility, the total solid solubility, and the emission rate correction are `SS.Factor`, `Total.SS.Factor`, and `Side.SS.Factor`, respectively.

## 4: Diffusion

### Dopant Diffusion in Silicon Germanium

---

## Germanium–Boron Pairing

Germanium can pair with boron and the pairs are known to be electrically active [27] but not mobile:



In Sentaurus Process, this reaction is modeled with the following differential equation:

$$\frac{\partial C_{GeB}}{\partial t} = Kf(C_{Ge}C_B - KbC_{GeB}) \quad (333)$$

where  $C_{GeB}$  is the concentration of germanium–boron pairs,  $C_{Ge}$  is the concentration of germanium,  $C_B$  is the concentration of boron, and  $Kf$  and  $Kb$  are the forward reaction rate and equilibrium constant, respectively.

You can specify the model parameters with the commands:

```
pdbSet Silicon Germanium Boron Kf {<n>}  
pdbSet Silicon Germanium Boron Kb {<n>}
```

Germanium diffusion is modeled by assuming a constant diffusion model:

$$\frac{\partial C_{Ge}}{\partial t} = \nabla \bullet (D \nabla C_{Ge}) \quad (334)$$

where  $D$  is the diffusivity of germanium and can be set using the command:

```
pdbSet Silicon Germanium Dstar {<n>}
```

**NOTE** The germanium–boron cluster model is switched off by default. To switch it on, use:

```
solution add name= GeB ifpresent= "Germanium Boron" !negative
```

Of course, if boron is present in silicon, the reaction in Eq. 333 is automatically added to Eq. 334.

Table 19 Solution names for germanium model

Symbol	Solution name
$C_{Ge}$	Germanium
$C_{GeB}$	GeB

## Initializing Germanium–Boron Clusters

Initially, germanium–boron cluster concentrations are set to zero. If there is an existing cluster concentration field, the field is used. To initialize the cluster concentration field, use the select command in the input command file.

---

## Diffusion in III–V Compounds

This section discusses diffusion in III–V compounds. For details on parameter interpolation, see [Alloy Materials and Parameter Interpolation on page 25](#).

---

## Converting Materials

When group III or group V atoms are doped into a III–V material, and the atoms are a different species from the components of the material, the material is converted to the new III–V material at the beginning of a diffuse command if the III–V material to be converted is in the Convert.Materials list for the converted III–V material:

```
pdbSet <converted_mat> Convert.Materials {<mat_to_beConverted list>}
```

For example:

```
pdbSet InGaAs Convert.Materials {GaAs}
```

specifies that a GaAs region will be converted to InGaAs at the beginning of a diffusion step under the following conditions:

- The Derived.Materials list of GaAs includes InGaAs:  

```
pdbSet GaAs Derived.Materials {InGaAs AlGaAs AlInGaAs}
```
- The maximum indium concentration in the region exceeds Min.Conv.Conc of indium for InGaAs:  

```
pdbSet InGaAs Indium Min.Conv.Conc 1E19
```

**NOTE** The diffusion model for alloy III–V materials requires correct material conversion. For example, GaAs doped with indium must be converted to InGaAs for the III–V diffusion model with mole fraction–dependent parameter values.

## 4: Diffusion

### Diffusion in III–V Compounds

---

## Merging Materials

When different III–V material regions are adjacent and there is a common material derived from each III–V material, the regions merge into the common derived material region at the beginning of a `diffuse` command if one of the neighbor materials has its neighbor material in the `Merge.Materials` list.

For example, if the neighbor region of a GaAs material region is InAs, two regions are merged and converted into InGaAs material if:

- The `Merge.Materials` list of GaAs (or InAs) includes InAs (or GaAs):

```
pdbSetString GaAs Merge.Materials {InAs}
```

- InGaAs is the derived material of both GaAs and InAs:

```
pdbSet GaAs Derived.Materials {InGaAs AlGaAs AlInGaAs}  
pdbSet InAs Derived.Materials {InGaAs AlInGaAs}
```

Likewise, InGaAs merges its neighbor GaAs (or InAs) if the `Merge.Materials` list of InGaAs includes GaAs (or InAs). When materials merge, the proper concentrations of the constituent atoms are allocated so that gallium atoms are doped ( $x=1.0$ ) in the GaAs region, and indium in InAs is also  $x=1.0$  in the InAs region.

---

## Dopant Diffusion

To model dopant diffusion in a III–V material, the following assumptions are applied:

- Point defects diffuse by the second nearest neighbor hopping.
- Group II dopants react only with group III point defects.
- Group VI dopants react only with group V point defects.
- There are no antisite defects.
- The charging reaction is in equilibrium.
- There are two types of vacancy (that is, at group III and V sites): `VacIII` and `VacV`.

Since the substitutional concentrations of group IV dopants on group III sites and group V sites are modeled and calculated separately, the autocompensation effect due to the amphoteric behavior is implicitly taken into account.

## ChargedReact Model

$$\frac{\partial AI}{\partial t} = \sum_m \left( \nabla \cdot \left( \left( \sum_j D_{AI_m j} \eta^{-j} \right) \eta^{-z_{Am}} \nabla \left( \frac{AI_m}{\alpha_{AI_m}} \eta^{z_{Am}} \right) \right) + \sum_{Y_m} R_{AY_m}^{(ko)} - R_{AIV_m}^{(ft)} \right) \quad (335)$$

$$\frac{\partial AV}{\partial t} = \sum_m \left( \nabla \cdot \left( \left( \sum_j D_{AV_m j} \eta^{-j} \right) \eta^{-z_{Am}} \nabla \left( \frac{AV_m}{\alpha_{AV_m}} \eta^{z_{Am}} \right) \right) + R_{AV_m}^{(ko)} - \sum_{Y_m} R_{AVY_m}^{(ft)} \right) \quad (336)$$

$$\frac{\partial A_{m,s}}{\partial t} = - \sum_{Y_m} R_{AY_m}^{(ko)} - R_{AV_m}^{(ko)} + R_{AIV_m}^{(ft)} + \sum_{Y_m} R_{AVY_m}^{(ft)} \quad (337)$$

where:

$$R_{AY_m}^{(ko)} = \left( \sum_j k_{AY_m j}^{(ko)} Y_{m,i}^* \phi_{Y_m j} \eta^{-j} \right) \left( A_{m,s} \frac{Y_m}{Y_m^*} - \frac{AI_m}{\alpha_{AI_m}} \frac{Y_{m,s}}{Y_{m,s}^*} \right) \quad (338)$$

$$R_{AV_m}^{(ko)} = \left( \sum_j k_{AV_m j}^{(ko)} V_{m,i}^* \phi_{V_m j} \eta^{-j} \right) \left( A_{m,s} \frac{V_m}{V_m^*} - \frac{AV_m}{\alpha_{AV_m}} \right) \quad (339)$$

$$R_{AIV_m}^{(ft)} = \left( \sum_{j,k} k_{AIV_m j k}^{(ft)} \alpha_{AI_m,j} V_{m,i}^* \phi_{V_m k} \eta^{-(j+k)} \right) \left( \frac{AI_m}{\alpha_{AI_m}} \frac{V_m}{V_m^*} - A_{m,s} \right) \quad (340)$$

$$R_{AVY_m}^{(ft)} = \left( \sum_{j,k} k_{AV_m j k}^{(ft)} \alpha_{AV_m,j} Y_{m,i}^* \phi_{Y_m k} \eta^{-(j+k)} \right) \left( \frac{AV_m}{\alpha_{AV_m}} \frac{Y_m}{Y_m^*} - A_{m,s} \frac{Y_{m,s}}{Y_{m,s}^*} \right) \quad (341)$$

$$\alpha_{AI_m} = \sum_j \alpha_{AI_m,j} \eta^{-j} \text{ and } \alpha_{AI_m,j} \equiv D_{AI_m j} / d_{AI_m j} \quad (342)$$

$$\alpha_{AV_m} = \sum_j \alpha_{AV_m,j} \eta^{-j} \text{ and } \alpha_{AV_m,j} \equiv D_{AV_m j} / d_{AV_m j} \quad (343)$$

$$AI_{III} = \frac{\alpha_{AI_{III}} \eta^{-1}}{\alpha_{AI_{III}} \eta^{-1} + \alpha_{AI_V} \eta^1 / r_{III V}} AI \quad (344)$$

$$AI_V = \frac{\alpha_{AI_V} \eta^1}{r_{III V} \alpha_{AI_{III}} \eta^{-1} + \alpha_{AI_V} \eta^1} AI \quad (345)$$

## 4: Diffusion

### Diffusion in III–V Compounds

$$AV_{III} = \frac{\alpha_{AV_{III}} \eta^{-1}}{\alpha_{AV_{III}} \eta^{-1} + \alpha_{AV_V} \eta^1 / r_{III\bar{V}}} AV \quad (346)$$

$$AV_V = \frac{\alpha_{AV_V} \eta^1}{r_{III\bar{V}} \alpha_{AV_{III}} \eta^{-1} + \alpha_{AV_V} \eta^1} AV \quad (347)$$

Table 20 Description of symbols for the ChargedReact model

Symbol	Description	Unit
$m$	The Mendeleev group number of a constituent atom of III–V material, $m \in \{III, V\}$ .	Unitless
$A_{m,s}$	Substitutional dopant concentration at group $m$ lattice sites.	$\text{cm}^{-3}$
$AI$	Dopant–interstitial pair concentration. For example, $AI$ is SiInt for Silicon.	$\text{cm}^{-3}$
$AI_m$	Dopant–group $m$ interstitial pair concentration.	$\text{cm}^{-3}$
$AV$	Dopant–vacancy pair concentration. For example, $AV$ is SiVac for Silicon.	$\text{cm}^{-3}$
$AV_m$	Dopant–group $m$ vacancy pair concentration.	$\text{cm}^{-3}$
$Y_m$	Self-interstitial concentration. For example, $Y_{III}$ is GaInt or InInt, and $Y_V$ is AsInt in InGaAs.	$\text{cm}^{-3}$
$Y_{m,s}$	Constituent atom concentration. For example, $Y_{III,s}$ is Gallium or Indium, and $Y_V$ is Arsenic in InGaAs.	$\text{cm}^{-3}$
$Y_m^*$	Self-interstitial concentration in equilibrium (Eq. 361, p. 257).	$\text{cm}^{-3}$
$Y_{m,i}^*$	Self-interstitial concentration in intrinsic equilibrium: The interpolated value is used unless users specify the value for the alloy, for example: pdbSet InGaAs GaInt Cstar {<n>}	$\text{cm}^{-3}$
$Y_{m,s}^*$	Constituent atom concentration in equilibrium: pdbSet InGaAs Gallium CsubStar {<n>}	$\text{cm}^{-3}$
$\phi_{Y_m}$	Charge-state fractions of self-interstitials: $\phi_{Y_{mj}} = \phi_{Y_{mj}}' / \sum_j \phi_{Y_{mj}}' \cdot \phi_{Y_{mj}}'$ is specified, for example, by: pdbSet GaAs GaInt ChargeStates {-2 <n> ... 2 <n>}	Unitless
$V_m$	Vacancy concentration. $V_{III}$ is VacIII and $V_V$ is VacV.	$\text{cm}^{-3}$
$V_m^*$	Vacancy concentration in equilibrium (Eq. 362, p. 257).	$\text{cm}^{-3}$
$V_{m,i}^*$	Vacancy concentration in intrinsic equilibrium: pdbSet GaAs VacIII Cstar {<n>}	$\text{cm}^{-3}$
$\phi_{V_m}$	Charge-state fractions of vacancies: $\phi_{V_{mj}} = \phi_{V_{mj}}' / \sum_j \phi_{V_{mj}}' \cdot \phi_{V_{mj}}'$ is specified, for example, by: pdbSet GaAs VacIII ChargeStates {-2 <n> ... 2 <n>}	Unitless

Table 20 Description of symbols for the ChargedReact model

Symbol	Description	Unit
$D_{AI_m}$	Effective diffusivity of dopant–group $m$ interstitial: pdbSet <mat> <dopant> IntIII D { -2 <n> ... 2 <n> } pdbSet <mat> <dopant> IntV D { -2 <n> ... 2 <n> }	$\text{cm}^2/\text{s}$
$D_{AV_m}$	Effective diffusivity of dopant–group $m$ vacancy: pdbSet <mat> <dopant> VacIII D { -2 <n> ... 2 <n> } pdbSet <mat> <dopant> VacV D { -2 <n> ... 2 <n> }	$\text{cm}^2/\text{s}$
$d_{AI_m}$	Self-diffusivity of dopant–group $m$ interstitial: pdbSet <mat> <dopant> IntIII Dpair { -2 <n> ... 2 <n> } pdbSet <mat> <dopant> IntV Dpair { -2 <n> ... 2 <n> }	$\text{cm}^2/\text{s}$
$d_{AV_m}$	Self-diffusivity of dopant–group $m$ vacancy: pdbSet <mat> <dopant> VacIII Dpair { -2 <n> ... 2 <n> } pdbSet <mat> <dopant> VacV Dpair { -2 <n> ... 2 <n> }	$\text{cm}^2/\text{s}$
$\alpha_{AI_m}$	Ratio of dopant–group $m$ interstitial pair concentration to substitutional concentration in equilibrium.	Unitless
$\alpha_{AV_m}$	Ratio of dopant–group $m$ vacancy pair concentration to substitutional concentration in equilibrium.	Unitless
$z_{Am}$	Charge of ionized substitutional atom at group $m$ lattice sites.	Unitless
$\eta$	Ratio of electron concentration to intrinsic carrier concentration ( $n/n_i$ ).	Unitless
$R_{AY_m}^{(ko)}$	Kick-out reaction rate at which $Y_m$ kicks out $A_{m,s}$ , generates $AI_m$ , and increases the mole fraction of $Y$ .	$\text{cm}^{-3}/\text{s}$
$R_{AV_m}^{(ko)}$	Kick-out reaction rate at which $V_m$ reacts with $A_{m,s}$ and generates a dopant–vacancy pair $AV_m$ .	$\text{cm}^{-3}/\text{s}$
$R_{AIV_m}^{(ft)}$	Frank–Turnbull reaction rate at which $AI_m$ reacts with $V_m$ and generates a substitutional dopant $A_{m,s}$ .	$\text{cm}^{-3}/\text{s}$
$R_{AVY_m}^{(ft)}$	Frank–Turnbull reaction rate at which $AV_m$ reacts with $Y_m$ , generates a substitutional dopant $A_{m,s}$ , and increases the mole fraction of $Y$ .	$\text{cm}^{-3}/\text{s}$
$k_{AY_m}^{(ko)}$	Reaction rate constant associated with $R_{AY_m}^{(ko)}$ , for example: pdbSet GaAs Si Gallium kfKickOut { -2 <n> ... 2 <n> }	$\text{cm}^{-3}/\text{s}$
$k_{AV_m}^{(ko)}$	Reaction rate constant associated with $R_{AV_m}^{(ko)}$ , for example: pdbSet GaAs Si VacV kfKickOut { -2 <n> ... 2 <n> }	$\text{cm}^{-3}/\text{s}$
$k_{AIV_m}^{(ft)}$	Reaction rate constant associated with $R_{AIV_m}^{(ft)}$ , for example: pdbSet GaAs Si VacIII kfFTM { {-2,-2} <n> ... {2,2} <n> }	$\text{cm}^{-3}/\text{s}$
$k_{AVY_m}^{(ft)}$	Reaction rate constant associated with $R_{AVY_m}^{(ft)}$ , for example: pdbSet GaAs Si Gallium kfFTM { {-2,-2} <n> ... {2,2} <n> }	$\text{cm}^{-3}/\text{s}$

#### 4: Diffusion

##### Diffusion in III–V Compounds

Table 20 Description of symbols for the ChargedReact model

Symbol	Description	Unit
$r_{III\text{V}}$	Ratio of the substitutional concentration at group III lattice sites to group V sites in intrinsic equilibrium. $r_{III\text{V}} \equiv (A_{III,s}/A_{V,s})_i^*$ . Applies only to group IV dopants. For example: pdbSet GaAs Si Csub.Ratio {<n>}	Unitless

## Fermi Model

The point-defect concentrations are assumed to be at thermal equilibrium:

$$\frac{\partial A}{\partial t} = \sum_m \nabla \cdot \left( (D_{I_m} + D_{V_m}) \eta^{-z_m} \nabla (A_{m,s} \eta^{z_m}) \right) \quad (348)$$

where:

$$A_{III,s} = \frac{\eta^{-1}}{\eta^{-1} + \eta^1 / r_{III\text{V}}} A_s \quad (349)$$

$$A_{V,s} = \frac{\eta^1}{r_{III\text{V}} \eta^{-1} + \eta^1} A_s \quad (350)$$

## Constant Model

The point-defect concentrations are assumed to be at intrinsic equilibrium:

$$\frac{\partial A}{\partial t} = \sum_m \nabla \cdot (D^* \nabla (A_{m,s})) \quad (351)$$

where:

$$A_{III,s} = \frac{1}{1 + 1/r_{III\text{V}}} A_s \quad (352)$$

$$A_{V,s} = \frac{1}{r_{III\text{V}} + 1} A_s \quad (353)$$

---

## Activation Model

The solid solubility model can be specified. For more information, see [Dopant Active Model: Solid on page 277](#). For group IV dopants, the amount of substitutional concentration on group III and group V sites is reduced by the ratio of a given parameter `Csub.Clust.Ratio` to the clustering concentration, respectively:

$$A_{III,s}^+ = A_{III,s} - \frac{1}{1 + 1/C_{sub.Clust.Ratio}} (A_s - A_s^+) \quad (354)$$

$$A_{V,s}^+ = A_{V,s} - \frac{1}{C_{sub.Clust.Ratio} + 1} (A_s - A_s^+) \quad (355)$$

---

## Point-Defect Diffusion

$$\frac{\partial Y_m}{\partial t} = \nabla \cdot \left( \left( \sum_j d_{Y_m,j} Y_{m,i}^* \phi_{Y_m,j} \eta^{-j} \right) \nabla \left( \frac{Y_m}{Y_m^*} \right) \right) - R_{YV_m} - \sum_{Y'_m} R_{YY'_m} - \sum_A (R_{AY_m}^{(ko)} + R_{AVY_m}^{(ft)}) \quad (356)$$

$$\frac{\partial V_m}{\partial t} = \nabla \cdot \left( \left( \sum_j d_{V_m,j} V_{m,i}^* \phi_{V_m,j} \eta^{-j} \right) \nabla \left( \frac{V_m}{V_m^*} \right) \right) - \sum_{Y_m} R_{YV_m} - \sum_A (R_{AV_m}^{(ko)} + R_{AIV_m}^{(ft)}) \quad (357)$$

$$\frac{\partial Y_{m,s}}{\partial t} = R_{YV_m} + \sum_{Y'_m} R_{YY'_m} + \sum_A (R_{AY_m}^{(ko)} + R_{AVY_m}^{(ft)}) \quad (358)$$

where:

$$R_{YV_m} = \left( \sum_{j,k} k_{YV_m,j} (Y_{m,i}^* \phi_{Y_m,j}) (V_{m,i}^* \phi_{V_m,k}) \eta^{-(j+k)} \right) \left( \frac{Y_m}{Y_m^*} \frac{V_m}{V_m^*} - \frac{Y_{m,s}}{Y_{m,s}^*} \right) \quad (359)$$

$$R_{YY'm} = \left( \sum_j k_{YY'_m,j} Y'_{m,s}^* (Y_{m,i}^* \phi_{Y_m,j}) \eta^{-j} \right) \left( \frac{Y_m}{Y_m^*} \frac{Y'_{m,s}}{Y'_{m,s}^*} - \frac{Y'_{m,s}}{Y'_{m,s}^*} \right) \quad (360)$$

$$Y_m^* = \sum_j Y_{m,i}^* \phi_{Y_m,j} \eta^{-j} \quad (361)$$

$$V_m^* = \sum_j V_{m,i}^* \phi_{V_m,j} \eta^{-j} \quad (362)$$

## 4: Diffusion

### Diffusion in III–V Compounds

Table 21 Description of symbols for the pair diffusion model

Symbol	Description	Unit
$m$	The Mendeleev group number of a constituent atom of III–V material, $m \in \{III, V\}$ .	Unitless
$Y_m$	Self-interstitial concentration. For example, $Y_{III}$ is GaInt or InInt, and $Y_V$ is AsInt in InGaAs.	$\text{cm}^{-3}$
$Y_{m,s}$	Constituent atom concentration. For example, $Y_{III,s}$ is Gallium or Indium, and $Y_V$ is Arsenic in InGaAs.	$\text{cm}^{-3}$
$Y_m^*$	Self-interstitial concentration in equilibrium (Eq. 361, p. 257).	$\text{cm}^{-3}$
$Y_{m,i}^*$	Self-interstitial concentration in intrinsic equilibrium: pdbSet InGaAs GaInt Cstar {<n>}	$\text{cm}^{-3}$
$Y_{m,s}^*$	Constituent atom concentration in equilibrium: pdbSet InGaAs Gallium CsubStar {<n>}	$\text{cm}^{-3}$
$\phi_{Y_m}$	Charge-state fractions of self-interstitials: $\phi_{Y_mj} = \phi_{Y_mj}' / \sum_j \phi_{Y_mj}' \cdot \phi_{Y_mj}'$ is specified, for example, by: pdbSet GaAs GaInt ChargeStates { -2 <n> ... 2 <n> }	Unitless
$V_m$	Vacancy concentration. $V_{III}$ is VacIII and $V_V$ is VacV.	$\text{cm}^{-3}$
$V_m^*$	Vacancy concentration in equilibrium (Eq. 362, p. 257).	$\text{cm}^{-3}$
$V_{m,i}^*$	Vacancy concentration in intrinsic equilibrium: pdbSet GaAs VacIII Cstar {<n>}	$\text{cm}^{-3}$
$\phi_{V_m}$	Charge-state fractions of vacancies: $\phi_{V_mj} = \phi_{V_mj}' / \sum_j \phi_{V_mj}' \cdot \phi_{V_mj}'$ is specified, for example, by: pdbSet GaAs VacIII ChargeStates { -2 <n> ... 2 <n> }	Unitless
$d_{Ym}$	Self-interstitial diffusivity: pdbSet InGaAs GaInt D { -2 <n> ... 2 <n> }	$\text{cm}^2/\text{s}$
$d_{Vm}$	Vacancy diffusivity: pdbSet GaAs VacIII D { -2 <n> ... 2 <n> }	$\text{cm}^2/\text{s}$
$\eta$	Ratio of electron concentration to intrinsic carrier concentration ( $n/n_i$ ).	Unitless
$R_{AY_m}^{(ko)}$	Kick-out reaction rate at which $Y_m$ kicks out $A_{m,s}$ , generates $AI_m$ , and increases the mole fraction of $Y$ . See Eq. 338, p. 253 for details.	$\text{cm}^{-3}/\text{s}$
$R_{AV_m}^{(ko)}$	Kick-out reaction rate at which $Y_m$ reacts with $A_{m,s}$ and generates a dopant–vacancy pair $AV_m$ . See Eq. 339, p. 253 for details.	$\text{cm}^{-3}/\text{s}$
$R_{AIV_m}^{(ft)}$	Frank–Turnbull reaction rate at which $AI_m$ reacts with $V_m$ and generates a substitutional dopant $A_{m,s}$ . See Eq. 340, p. 253 for details.	$\text{cm}^{-3}/\text{s}$
$R_{AVY_m}^{(ft)}$	Frank–Turnbull reaction rate at which $AV_m$ reacts with $Y_m$ , generates a substitutional dopant $A_{m,s}$ , and increases the mole fraction of $Y$ . See Eq. 341, p. 253 for details.	$\text{cm}^{-3}/\text{s}$
$R_{YV_m}$	Interstitial–vacancy bulk recombination rate for group $m$ .	$\text{cm}^{-3}/\text{s}$

Table 21 Description of symbols for the pair diffusion model

Symbol	Description	Unit
$R_{YY'_m}$	Kick-out reaction rate at which $Y_m$ kicks out $Y_{m,s}$ and occupies the lattice site by generating $Y'_m$ . The reaction increases the mole fraction of $Y$ but decreases that of $Y'$ .	$\text{cm}^{-3}/\text{s}$
$k_{YY'_m}$	Reaction rate constant associated with $R_{YY'_m}$ , for example: <code>pdbSet GaAs GaInt KbulkChargeStates { -2 &lt;n&gt; ... 2 &lt;n&gt; }</code>	$\text{cm}^{-3}/\text{s}$
$k_{YY'_m}$	Reaction rate constant associated with $R_{YY'_m}$ , for example: <code>pdbSet InGaAs GaInt Indium kfKickOut { -2 &lt;n&gt; ... 2 &lt;n&gt; }</code>	$\text{cm}^{-3}/\text{s}$

## Poisson Equation

$$\begin{aligned}
 & \nabla \bullet (\epsilon_r \epsilon_0 \nabla (\psi - \theta)) \\
 = & -q \left( p - n + \sum_A \sum_m (z_{Am} A_{m,s}) + \sum_A \sum_m \left( \left( \sum_j ((z_{Am} + j) \alpha_{AI_m,j} \eta^{-j}) \right) \frac{AI_m}{\alpha_{AI_m}} + \left( \sum_j ((z_{Am} + j) \alpha_{AV_m,j} \eta^{-j}) \right) \frac{AV_m}{\alpha_{AV_m}} \right) \right. \\
 & \left. + \sum_m \left( \sum_j \left( \sum_i j Y_{m,i} * \phi_{Y_m,j} \eta^{-j} \right) \frac{Y_m}{Y_m^*} + \left( \sum_j j V_{m,i} * \phi_{V_m,j} \eta^{-j} \right) \frac{V_m}{V_m^*} \right) \right) \tag{363}
 \end{aligned}$$

The band structure parameter  $\theta$  (Eq. 373, p. 262) relies on the mole fraction-dependent affinity and the energy bandgap (see [Poisson Equation for Heterojunctions on page 262](#)).

## Pressure-Dependent Defect Diffusion

[Eq. 142, p. 183](#) shows that  $C_X^*$  depends on the Fermi level. However, you can select one of the available models using the command:

```
pdbSet <material> <defect> CStarMod <model>
```

where:

- `<defect>` is interstitial or vacancy.
- `<model>` is one of the following models: Constant, FermiLevelDependent, or FermiPressureDependent.

The Constant model simply sets  $C_X^*$  to  $C_{X(intrinsic)}^*$ , the FermiLevelDependent model is given in [Eq. 142](#), and the FermiPressureDependent model includes both Fermi effects and pressure-field effects.

The pressure effects are modeled in Sentaurus Process by modifying the equilibrium point-defect concentrations:

$$C_X^* = C_X^*(Si, P=0) e^{-\frac{(\Delta V_X P)}{kT}} \quad (364)$$

where  $C_X^*$  is the total equilibrium concentration of point defect  $X$  (interstitial or vacancy).  $\Delta V_X$  is the activation volume change of equilibrium point defects due to the pressure  $P$  and is given by:

$$\Delta V_I = \epsilon 4\pi r_o^3 \quad (365)$$

$$\Delta V_V = -2\pi r_s^2 3 \frac{(1-\eta)}{1+\eta} \frac{\Gamma}{\mu} \quad (366)$$

where  $\epsilon$  is the dilatation,  $r_o$  is the measure of the sphericity of the interstitial,  $r_s$  is the radius of the vacancy,  $\eta$  is the Poisson ratio of silicon,  $\Gamma$  is the surface tension of the vacancy, and  $\mu$  is the shear modulus of silicon. The following set of commands can be used to modify  $\Delta V_X$ :

```
pdbSet Silicon Interstitial Volume 8.59e-24
pdbSet Silicon Vacancy Volume -5.52e-24
```

The unit of Volume is cm<sup>3</sup>.

## Electron Concentration

To calculate the electron concentration or, alternatively, the electron potential, Sentaurus Process solves either the Poisson equation or charge balance equation in semiconductors such as silicon, germanium, and polysilicon. By default, the ChargedReact, ChargedPair, and ChargedEquilibrium models all solve the charge balance equation. The uncharged models do not require a separate equation because the electron concentration can be computed directly from the net doping.

The Poisson equation is given by:

$$\nabla \bullet (\epsilon \nabla \psi) = -q(p - n + \Delta N) \quad (367)$$

where  $\epsilon$  is the permittivity,  $\psi$  is the potential,  $n$  and  $p$  are the electron and hole concentrations, and  $\Delta N$  is the net charge.

Electrons and holes are always assumed to be in equilibrium, such that:

$$pn = n_i^2 \quad (368)$$

The charge balance equation is:

$$-n + p + \Delta N = 0 \quad (369)$$

In [Eq. 367](#) and [Eq. 369](#), the  $\Delta N$  must be calculated. The net charge is given by:

$$\Delta N = \sum_j z_j C_{A_j}^+ + \sum_c c C_{X^c} + \sum_{X, c, j} (z_j + c) C_{A_j X}^{(c + z_j)} \quad (370)$$

where:

- $c$  is the charge state of the defect  $X$ , interstitial, or vacancy.
- $C_{X^c}$  is the concentration of the defect  $X$  in the charge state  $c$ .
- $z_j$  is the charge state of dopant  $A_j$ .
- $A_j X$  is the dopant  $A_j$  and defect  $X$  pair.

You can exclude or include the charged dopant–defect pairs or charged defects in [Eq. 370](#), for example:

```
pdbSet Si Dopant ChargeModel DopantOnly
pdbSet Si Dopant ChargeModel DopantDefect
```

The first command, which is the default behavior for dopants, includes only the charged dopants in silicon in [Eq. 370](#). The second command includes the charged dopants as well as the charged dopant–defect pairs in [Eq. 370](#).

In a similar way:

```
pdbSet Si Defect ChargeModel None
pdbSet Si Defect ChargeModel Defect
```

The first command, which is the default behavior for defects, excludes the charged defects in silicon in [Eq. 370](#) and the second command includes them.

**NOTE** The diffusion models Constant, Fermi, Pair, and React always exclude the charged dopant–defect pairs.

The Poisson equation is switched on or off with the command:

```
pdbSet Si Potential Poisson <1 | 0>
```

**NOTE** The above switch is used to change from the Poisson equation to the charge balance equation, and vice versa.

If it is switched off, the charged defects and charged dopant–defect pairs are not included in Eq. 370, and Eq. 371 is used to calculate the potential:

$$\psi = \frac{1}{V_{ti}} \log \left( \frac{1}{2n_i} (\Delta N + \sqrt{\Delta N^2 + 4n_i^2}) \right) \quad (371)$$

where  $V_{ti}$  is  $1/kT$ , and  $n_i$  is the intrinsic concentration of electrons and can be set using the command:

```
pdbSet <material> Potential ni {<n>}
```

To switch on or off the solution of the Poisson equation or the charge balance equation, regardless of the diffusion model selected, use the commands:

```
pdbSetBoolean Potential ForcedTurnOff <0 | 1>
pdbSetBoolean Potential ForcedTurnOn <1 | 0>
```

**NOTE** If the potential equation is switched off, charge neutrality is assumed. If the selected diffusion or cluster models use complex charges, this may lead to instability in the code.

## Poisson Equation for Heterojunctions

A heterojunction is the interface that occurs between two layers or regions of dissimilar crystalline semiconductors. At the interface, the behavior of a semiconductor junction depends strongly on the alignment of the energy bands. The different electron affinity or the energy bandgap causes the electron pileup or depletion, which affects the dopant diffusion. The Poisson equation for heterojunctions is given by:

$$\nabla \bullet (\epsilon_r \epsilon_0 \nabla (\psi - \theta)) = -q(p - n + \Delta N) \quad (372)$$

where:

$$q\theta = \chi + \frac{E_g}{2} + \frac{kT}{2} \ln \left( \frac{N_c}{N_v} \right) \quad (373)$$

$$n = n_i \exp \left( \frac{q\psi}{kT} \right) \text{ and } p = n_i \exp \left( -\frac{q\psi}{kT} \right) \quad (374)$$

$$N_c = N_{c300} \left( \frac{T}{300} \right)^{3/2} \quad (375)$$

$$N_v = N_{v300} \left( \frac{T}{300} \right)^{3/2} \quad (376)$$

$$n_i = \sqrt{N_c N_v} \exp\left(-\frac{E_g}{2kT}\right) \quad (377)$$

$$E_g = E_{g300} + E_{g\alpha} \left( \frac{300^2}{300 + \beta} - \frac{T^2}{T + \beta} \right) \quad (378)$$

Table 22 Description of symbols for Poisson equation

Symbol	Description	Unit
$\Psi$	Intrinsic Fermi potential.	V
$\theta$	Band structure parameter.	V
$\epsilon_0$	Vacuum permittivity ( $8.854 \times 10^{-12}$ F/m).	F/m
$\epsilon_r$	Relative permittivity: pdbSet <material> Potential Permittivity {<n>}	Unitless
$\eta$	Ratio of electron concentration to intrinsic carrier concentration ( $n/n_i$ ).	Unitless
$\chi$	Affinity that depends on the mole fraction $x$ : pdbSet <material> Potential Affinity {<n>}	eV
$E_{g300}$	Band gap at 300 K, which depends on the mole fraction $x$ : pdbSet <material> Potential Eg300 {<n>}	eV
$E_{g\alpha}$	Bandgap modification for temperature dependency: pdbSet <material> Potential Eg.Alpha {<n>}	eV
$\beta$	Temperature constant for band gap depending on temperature: pdbSet <material> Potential Eg.Beta {<n>}	K
$N_c$	Density-of-states of a conduction band.	$\text{cm}^{-3}$
$N_{c300}$	Density-of-states of a conduction band at 300 K: pdbSet <material> Potential Nc300 {<n>}	$\text{cm}^{-3}$
$N_v$	Density-of-states of a valence band.	$\text{cm}^{-3}$
$N_{v300}$	Density-of-states of a valence band at 300 K: pdbSet <material> Potential Nv300 {<n>}	$\text{cm}^{-3}$

Switching on Use.DOS specifies using the density-of-states to calculate the intrinsic carrier concentration. If Use.DOS is switched off,  $\theta$  is set to 0.0 and  $n_i$  is given by the PDB parameter ni:

```
pdbSet Silicon Potential Use.DOS 0
```

## 4: Diffusion

### Electron Concentration

To solve the Poisson equation in insulators or to apply Dirichlet boundary conditions at conductor surfaces, use:

```
pdbSet <material> Potential Poisson 1
```

For example:

```
pdbSet Oxide Potential Poisson 1  
pdbSet Aluminum Potential Poisson 1
```

**NOTE** Dirichlet boundary conditions are applied automatically to metal-insulator or metal-semiconductor interfaces only when the Poisson equation is switched on in both neighboring materials.

**NOTE** Continuous boundary conditions are applied automatically to insulator-insulator, insulator-semiconductor, and semiconductor-semiconductor interfaces only when the Poisson equation is switched on in both neighboring materials.

To define a conductor, set the Conductor and WorkFunction parameters. For example:

```
pdbSet Aluminum Conductor 1  
pdbSet Aluminum Potential WorkFunction 4.1
```

Table 23 Default conductor materials and their workfunctions

Material	Workfunction [eV]
Aluminum	4.10
Cobalt	5.00
CobaltSilicide	4.76
Copper	4.70
Nickel	5.20
NickelSilicide	4.84
Platinum	5.50
TiSilicide	4.56
Titanium	4.33
Tungsten	4.80
TungstenSilicide	4.76

To switch on the Poisson equation for all material regions in a simulation structure, use:

```
pdbSet Compute All.Poisson 1
```

## Bandgap Narrowing

If bandgap narrowing effects must be considered, Sentaurus Process uses the effective intrinsic electron density ( $n_{ie}$ ) instead of  $n_i$ .  $n_{ie}$  is given by:

$$n_{ie} = n_i e^{-\frac{\Delta E_g}{2kT}} \quad (379)$$

where  $\Delta E_g$  is the reduction in the bandgap energy of silicon and is defined as:

$$\Delta E_g = \Delta E_{gu} + \Delta E_{gs} \quad (380)$$

where  $\Delta E_{gu}$  is the user-defined bandgap narrowing and can be set using:

```
 pdbSet <material> Potential delEg {<n>}
```

$\Delta E_{gs}$  is the bandgap narrowing due to strain in the structure. To switch on this effect, the intrinsic electron density model (niMod) must be set to StrainDependent. To select the model, use:

```
 pdbSet <material> Potential niMod {Constant | StrainDependent}
```

If the Constant model is selected, it will ignore  $\Delta E_{gs}$ .

If the StrainDependent model is selected,  $\Delta E_{gs}$  will be calculated [28] using:

$$\Delta E_{ci} = D_{ci}(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) + D_{cxi}\epsilon_{xx} + D_{cyi}\epsilon_{yy} + D_{czi}\epsilon_{zz} \quad (381)$$

$$\begin{aligned} \Delta E_{vi} &= D_{vi}(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) \\ &\pm \sqrt{(0.5D_{vbi}^2((\epsilon_{xx} - \epsilon_{yy})^2 + (\epsilon_{yy} - \epsilon_{zz})^2 + (\epsilon_{zz} - \epsilon_{xx})^2) + D_{vdi}^2(\epsilon_{xy}^2 + \epsilon_{xz}^2 + \epsilon_{yz}^2))} \end{aligned} \quad (382)$$

where  $\epsilon$  is the strain in the respected direction, and  $D_{ci}$ ,  $D_{vi}$  are the dilatational deformation potentials for the conduction and valence band valleys, respectively.

To set, use:

```
 pdbSet Silicon Potential Ec Dilatational { 1 -8.6
                                            2 -8.6
                                            3 -8.6 }
 pdbSet Silicon Potential Ev Dilatational { 1 -2.1
                                            2 -2.1 }
```

## 4: Diffusion

### Electron Concentration

$D_{cxi}, D_{cyi}, D_{czi}$  and  $D_{vbi}, D_{vdi}$  are the deviatoric deformation potential of conduction and valence band valleys. They can be set using the commands:

```

pdbSet Si Potential Ec Deviatoric(1) { 1 9.5
                                         2 0.0
                                         3 0.0 }
pdbSet Si Potential Ec Deviatoric(2) { 1 0.0
                                         2 9.5
                                         3 0.0 }
pdbSet Si Potential Ec Deviatoric(3) { 1 0.0
                                         2 0.0
                                         3 9.5 }
pdbSet Si Potential Ev Deviatoric(1) { 1 0.5
                                         2 4.0 }
pdbSet Si Potential Ev Deviatoric(2) { 1 0.5
                                         2 4.0 }

```

Sentaurus Process uses the averaged values of the conduction band and valence band energies,  $\Delta Eci, \Delta Evi$ :

$$\Delta Ec = -kT \log \left( \frac{1}{3} \sum_{i=1}^3 e^{-\frac{\Delta Eci}{kT}} \right) \quad (383)$$

$$\Delta Ev = kT \log \left( \frac{1}{2} \sum_{i=1}^2 e^{-\frac{\Delta Evi}{kT}} \right) \quad (384)$$

This approach assumes that the mechanical strain keeps the densities-of-states unchanged in each subband of an initially degenerated band extremum, producing only the splitting of the subbands, thereby changing the effective band-edge position. In addition, the effective densities-of-states are assumed to be equal among the three conduction-band minima and among the two valence-band (light hole and heavy hole) maxima. The bandgap narrowing becomes:

$$\Delta Egs = \Delta Ec - \Delta Ev \quad (385)$$

If `Use.DOS` is switched on and `niMod` is `StrainDependent`, stress corrections  $\Delta Eci, \Delta Egs$  are included in the computation of terms  $\theta$  and  $n_i$  using the corrections of  $\chi$  and  $E_g$  (see [Eq. 373, p. 262](#) and [Eq. 377, p. 263](#)).

**NOTE**  $\Delta Egs$  is ignored in silicon-like materials where  $Ge/5e22 > 0.1\%$ , when parameter interpolation is not used and the default PDB parameter `<material> Germanium delEg { [GedelEg] }` is used together with the default procedure `GedelEg` (see [Dopant Diffusion in Silicon Germanium on page 241](#)).

---

## Epitaxy

Epitaxial growth is simulated when an `Epi` type ambient is specified in either the `diffuse` command or a `temp_ramp` ramp used by the `diffuse` command.

By default, two `Epi` type ambients are available: `Epi` and `LTE`. If `Epi` is specified, `Silicon` will grow on `Silicon` and `PolySilicon` will grow on `PolySilicon`. If `LTE` is specified, `Silicon` will again grow on `Silicon`, but `PolySilicon` will grow on `Oxide`, `Nitride`, and `PolySilicon`. The layer thickness is specified with the `thick` parameter and doping is specified with the `epi.doping` parameter.

Epitaxy is solved using the Alagator generic growth scheme (see [Basics of Specifying Generic Growth Equations on page 612](#)). This allows you to introduce new materials and material-dependent growth rates.

An unlimited number of species can be incorporated into the epitaxial layer. Doping is specified using the `epi.doping` and `epi.doping.final` parameters in either the `diffuse` command or a `temp_ramp` included in a `diffuse` command. The parameters `<material> <solution> Cepi0` and `<material> <solution> CepiE` set the default value of fields in the growing material. The defaults are overwritten by setting the `epi.doping` and `epi.doping.final` parameters of the `diffuse` or `temp_ramp` commands.

The same set of equations as for the single-crystalline silicon is solved for the epitaxial silicon during the diffusion step simulation. If the growth temperature decreases below the minimum diffusion temperature, the diffusion equations will be switched off, but the boundary conditions for dopant incorporation will be applied. In this case, the `Continuous` boundary condition is applied to all the mobile species at the interface between the epitaxial layer and single-crystalline silicon to take into account the variable jump.

It is also possible to incorporate dopants by auto-doping during the epitaxial growth using the `auto.doping` parameter in either the `diffuse` command or a `temp_ramp` included in a `diffuse` command. Auto-doping can be switched on only for dopants that are not listed in the `epi.doping` or `epi.doping.final` parameters (see [Epi Auto-Doping on page 269](#)).

In certain examples, it is easier to specify a resistivity of a required homogeneous doping level in the `epi` layer. The resistivity can be specified using the `epi.resist` parameter in either the `diffuse` command or a `temp_ramp` included in a `diffuse` command.

Different methods can be selected to simulate the epitaxial growth. The `epi.model` argument of the `diffuse` command is used to switch between them:

- `epi.model=0` (default) applies a moving-boundary algorithm similar to the oxidation one.
- `epi.model=1` uses alternating doped deposition and inert annealing steps. Model 1 supports selective epitaxy and material-dependent growth rates, and can be used with both

## 4: Diffusion

### Epitaxy

Sentaurus Structure Editor and the MGOALS module. For 3D epitaxy, Model 1 is recommended because of computational time and reliability issues related to moving boundaries (Model 0) in 3D simulations.

Both epitaxy models support graded doping. For `epi.model=0`, a correction towards grading is applied to boundary values for the solution fields that do not have any equation to be solved.

To set the grid spacing, use the `epi.layers` argument, which sets the number of grid layers that are deposited during the corresponding `diffuse` or `temp_ramp` steps.

**NOTE** Model 1 is recommended for 3D epitaxy and can be used with 2D.

---

## Using LKMC for Deposition Shape

The shape of the growing epi layer can be controlled by lattice kinetic Monte Carlo (LKMC) to obtain more realistic deposition shapes without having the performance penalty associated with the pure atomistic mode. To use this mode, specify `lkmc` in the `diffuse` command and the PDB parameter `KMC Epitaxy`, for example:

```
pdbSet KMC Epitaxy 1
diffuse time= 1<s> temperature= 550 Epi lkmc epi.thickness= 0.02
```

In this example, the LKMC epi growth rate is scaled such that the `<100>` direction (by default, the fastest direction) grows at  $0.02 \mu\text{m/s}$ . For more information about controlling LKMC epitaxy, see [Chapter 6 on page 567](#).

---

## Epi Doping

Two parameter lists of the `diffuse` and `temp_ramp` commands are used to control doping: `epi.doping` and `epi.doping.final`. Both lists take `<field>=<concentration>` elements as arguments.

If a dopant or field name appears in only one of the lists or in both lists with the same value, the value of the doping is constant throughout the step. If the dopant or field appears in both lists with different values, a linear gradient of the doping is applied by default. For example:

```
temp_ramp name= t1 temperature= 550 t.final= 700 time= 1<min>
temp_ramp name= t1 t.final= 700 time= 5<min> Epi thick= 0.1<um> \
    epi.doping= {Boron=1e18 Germanium=1e21} epi.doping.final= {Germanium=5e21}
diffuse temp.ramp= t1
```

In this example, epitaxy is simulated after an inert temperature ramp. During epitaxy, the boron concentration is a constant  $10^{18} \text{ cm}^{-3}$ , and germanium is ramped from  $10^{21} \text{ cm}^{-3}$  to

$5 \times 10^{21} \text{ cm}^{-3}$ . In addition, all these parameters can be set in the `diffuse` command, for example:

```
diffuse temperature= 700 time= 5<min> LTE epi.doping.final= {Arsenic=1e18} \
thick= 0.1<um>
```

In this case, a constant arsenic doping of  $10^{18} \text{ cm}^{-3}$  is incorporated in an LTE type of epitaxial growth.

## Initializing Dopant Clusters in Epi

The dopant cluster concentration in an epitaxial layer is initialized by:

$$\Delta C_{Aclust, i} = C_{Adoping, clust, i} + f_{Aclust, i} \cdot \max(C_{Adoping, dopant} - \text{EpiInit}, 0.0) \quad (386)$$

where  $f_{Aclust, i} = \frac{\text{FractionEpi}_i}{\sum \text{FractionEpi}_i}$ .

`EpiInit` and `FractionEpi` are specified by:

```
pdbSet <material> <dopant> EpiInit {<n>}
pdbSet <material> <cluster> FractionEpi {<n>}
```

The `epi.doping` list can include both a dopant and its cluster solutions, for example:

```
epi.doping= { Boron= 1e20 B4= 1e19 }
```

With `EpiInit=2×1019`, the concentrations of active boron (`Boron`) and  $\text{B}_4$  (`B4`) are set to  $2\times10^{19}$  and  $3\times10^{19}$  ( $(1\times10^{20} - 2\times10^{19})/4$ ), respectively.

## Epi Auto-Doping

The `auto.doping` argument of the `diffuse` and `temp_ramp` commands controls doping and takes a list of `<field>=<concentration>` elements as its value. If a dopant or field name appears in `auto.doping` and in either `epi.doping` or `epi.doping.final`, auto-doping of this dopant is ignored. For example:

```
temp_ramp name= t1 temperature= 550 t.final= 700 time= 1<min>
temp_ramp name= t1 t.final= 700 time= 5<min> Epi thick= 0.1<um> \
auto.doping= { Boron Germanium } epi.doping= { Germanium=1e21 }
diffuse temp.ramp= t1
```

## 4: Diffusion

### Epitaxy

In this example, only auto-doping of boron is simulated. The parameter `auto.doping` switches on the following phase transition (segregation) model automatically at Gas and epitaxially grown material interfaces:

$$\mathbf{j} \bullet \mathbf{n} = k_{Transfer} \left( \left( C_A^* e^{-\left( \frac{k_{Decay} \Delta t}{t} \right)} + C_A^{min} \right) - \frac{C_A}{k_{Segregation}} \right) \quad (387)$$

where  $k_{Transfer}$  is the transfer rate,  $k_{Segregation}$  is the segregation rate,  $C_A^*$  is the peak value of the dopant concentration in the auto-doped region,  $C_A^{min}$  is the minimum value of the dopant concentration,  $k_{Decay}$  is the decay rate of the auto-doping, and  $C_A$  is the dopant concentration. These parameters can be modified using the following commands, where `<interface_material>` is the Gas and epitaxially grown material interface:

```
pdbSet <interface_material> <dopant> TransferAutoDoping    <n>
pdbSet <interface_material> <dopant> SegregationAutoDoping <n>
pdbSet <interface_material> <dopant> Cstar                  <n>
pdbSet <interface_material> <dopant> minConc               <n>
pdbSet <interface_material> <dopant> DecayRate              <n>
```

In Eq. 387,  $\Delta t$  is the percentage of the simulation time since the diffusion started, and  $t$  is the total simulation time from the beginning to the end of diffusion. Eq. 387 is created automatically and stored in a term called `<dopant>AutoDoping`. You can overwrite this by defining your own reactions. For example:

```
term name=BoronAutoDoping EpiOnSilicon /Gas add eqn = \
"1e-3*(1e16-Boron_EpiOnSilicon/0.1)"
```

**NOTE** Since the model does not solve equations in gas, the dose loss or gain of the dopant is expected.

---

## Epi Doping Using Resistivity

The `epi.resist` parameter of the `diffuse` and `temp_ramp` commands controls doping. The parameter takes a list of parameters, that is, dopant name and resistivity, as its argument.

If more than one dopant name appears in the list, the doping concentration is calculated individually for each dopant by ignoring the other ones. For example:

```
temp_ramp name= t1 temperature= 550 t.final= 700 time= 1<min>
temp_ramp name= t1 t.final= 700 time= 5<min> Epi thick= 0.1<um> \
    epi.resist= { Arsenic=1e-2 Phosphorus=2e-3 }
diffuse temp.ramp= t1
```

In this example, epitaxy is simulated after an inert temperature ramp. During epitaxy, the active arsenic concentration and phosphorus concentration are calculated as  $4.3 \times 10^{19} \text{ cm}^{-3}$  and  $9.7 \times 10^{19} \text{ cm}^{-3}$ , respectively (see [Resistivity on page 879](#)). In addition, all of these parameters can be set in the `diffuse` command, for example:

```
diffuse temperature= 700 time= 5<min> LTE \
epi.resist= { Arsenic=1e-2 Phosphorus=2e-3 } thick= 0.1<um>
```

The doping concentration calculations use the silicon-based mobility models (see [Resistivity on page 879](#)).

---

## Epi Growth Settings: Low-Temperature Epitaxy

Several parameters are available for the simulation of effects seen in low-temperature epitaxy (LTE). LTE growth can result in the growth of polysilicon on insulators such as oxide and nitride after a seed layer has nucleated. In addition, the growth rate can depend on the starting material where the growth occurs. To allow different growth rates and nucleation times, Sentaurus Process uses temporary materials with distinct names that are converted back to standard names at the end of the `diffuse` command.

For example, during LTE, `LTEOnOxide` is grown on oxide, and `LTEOnSilicon` is grown on silicon (there are also the materials `LTEOnPolySilicon` and `LTEOnNitride`). After the diffusion step is completed, `LTEOnOxide` is converted to `PolySilicon`, and `LTEOnSilicon` is converted to `Silicon`.

**NOTE** Be aware that after material conversion, regions will merge if there are interfaces with the same material on both sides.

To set the nucleation delay for LTE growth on oxide, use:

```
pdbSet Gas_<starting_material> <ambient> NucleationDelay <n>
```

where `<n>` is the time in seconds. For the case of `LTEOnOxide`, `<starting_material>` is `Oxide` and `<ambient>` is `LTE`.

**NOTE** The *exposure time* is not saved, so nucleation must happen within one `diffuse` command (use the `temp_ramp` command to create long diffusion steps with optional ramp-up or ramp-down).

The growth rate for all materials is determined by default from the native layer thickness as well as the `thick` and `time` arguments of the `diffuse` command or the `temp_ramp` command. However, you can set the growth rate manually using a callback procedure like this:

```
pdbSet <growing_material>_Gas <ambient> GrowthRateProc <proc_name>
```

## 4: Diffusion

### Epitaxy

Inside <proc\_name>, you should set the pdb parameter GrowthReaction. For example:

```
pdbSet Gas_LTEOnOxide LTE GrowthRateProc MyGRProc
fproc MyGRProc { Mat Sol } {
    set myGrowthRate 1.0e-7          ;# in cm/s
    pdbSetString $Mat $Sol GrowthReaction "$myGrowthRate"
}
```

It is possible to set GrowthReaction to any Alagator expression not involving derivative expressions or element values.

---

## Simulating Facet Growth During Selective Epitaxy

To switch on faceting, use either:

- The angles.factors argument of the temp\_ramp (or diffuse) command.
- The PDB parameter <epimat gas interface> angles.factors along with setting the parameter pdbSet Grid AnisotropicGrowth 1.

The syntax for both angles.factors is similar:

```
temp_ramp angles.factors= {
    <interface material1>= { angle1(degrees) factor1(unitless)
                                angle2 factor2 ... }
    <interface material2>= { angle1(degrees) factor1(unitless)
                                angle2 factor2 ... }
    ...
}
```

or:

```
pdbSet <interface material> angles.factors {
    angle1(degrees) factor1(unitless) angle2 factor2 ...
}
```

where the interface material would be, for example, EpiOnSilicon\_Gas for epi growth on silicon and Gas\_LTEOnSilicon for LTE on silicon. There are aliases for all materials, so the order of the interface materials is not important.

To form facets, a large range of degrees near 0 that have a factor of 1.0 is needed. For larger angles, the factor should monotonously decrease to 0 at the required facet angle. For example, to form 35° facets during epi on silicon, the following setting could be used:

```
temp_ramp thick= <thick> epi time= <time> temperature= <temp> \
    epi.layers= <nlay> \
    angles.factors= { EpiOnSilicon_Gas= {0.0 1.0 20.0 1.0 35.0 0.0} }
```

## Controlling Where Facets Form

By default, facets form at all triple points (see [Triple-Point Control on page 673](#)). To switch off these facets, use:

```
pdbSet AnisoGrowthTriplePoints 0
```

By default, facets will not form on the outer boundaries. To switch on faceting on the outer boundary, use:

```
pdbSet AnisoGrowOuterBoundaries 1
```

## Time-Stepping

This algorithm and anisotropic growth in general can be inherently unstable. If a ‘bump’ develops during growth, it may persist or perhaps even grow larger. To prevent bumps from forming, it is necessary to take small time steps. The parameter `dThicknessAnisoGrowth` can be used to control time-stepping during anisotropic growth.

It sets a maximum thickness per time step:

```
pdbSet Diffuse dThicknessAnisoGrowth <thickness in um> #; default 0.001 um
```

## Other Effects on Dopant Diffusion

### Pressure-Dependent Dopant Diffusion

Dopant diffusivities can be enhanced or retarded due to stress or pressure. In addition to this, shrinking device dimensions can cause significant stress or pressure gradients affecting dopant diffusion further [\[28\]](#). With this model, Sentaurus Process allows diffusivities and gradients to be multiplied by user-defined factors as follows:

$$j = -DD_{SS}\nabla \frac{C}{D_{SP}} \quad (388)$$

where  $C$  is the concentration,  $D$  is the diffusivity, and  $D_{SS}$  and  $D_{SP}$  are user-definable terms. You can define both factors. To switch the model on or off, use the command:

```
pdbSet <material> <dopant> StressModel <model>
```

where `<model>` is either `None` (off, default) or `PDependent` (on).

For the definition of terms, see [Chapter 7 on page 603](#).

## 4: Diffusion

### Other Effects on Dopant Diffusion

For example, in the case of specified boron in silicon, this is given by:

```
term name=BoronIntSSFactor add Silicon eqn= {user-defined equation} store
term name=BoronIntSPFactor add Silicon eqn= {user-defined equation} store
```

To allow Sentaurus Process to use these terms, specify a term with the name <dopant><defect>SSFactor or <dopant><defect>SPFactor.

If the model is switched on and you do not provide the terms,  $D_{SS}$  and  $D_{SP}$  are calculated as:

$$D_{SS} = e^{-\frac{(\Delta V_V P)}{kT}} \quad (389)$$

$$D_{SP} = e^{-\frac{(\Delta V_S P)}{kT}} \quad (390)$$

where  $\Delta V_V$  and  $\Delta V_S$  are activation volumes and can be set using the commands:

```
pdbSet <material> <dopant> <defect> delVolV {<n>}
pdbSet <material> <dopant> <defect> delVols {<n>}
```

---

## Diffusion Prefactors

Dopant diffusivities can be enhanced or retarded due to various new process conditions. If a new model does not exist to simulate the observed behavior, you may want to multiply the existing diffusivity with a prefactor. Sentaurus Process allows diffusivities to be multiplied by user-defined factors as follows:

$$j = -DD_F \nabla C \quad (391)$$

where  $C$  is the concentration,  $D$  is the diffusivity, and  $D_F$  is the diffusion prefactor. For example, in the case of specified boron in silicon, this is given by:

```
term name= BoronDiffFactor add Silicon \
eqn= "exp(0.042 * $Vti * 125 * Germanium / 5e22)" store
```

The effective diffusivity of boron ( $D_B = D_{BI} + D_{BV}$ ) will be multiplied by BoronDiffFactor. (For the definition of terms, see [Using Terms on page 610](#).) Sentaurus Process also allows each dopant–defect diffusivity to be multiplied by a different user-defined factor:

$$j = -(D_{CI}D_{IF} + D_{CV}D_{VF}) \nabla C \quad (392)$$

where  $D_{CI}$  is the diffusivity of the dopant–interstitial pair,  $D_{CV}$  is the diffusivity of the dopant–vacancy pair, and  $D_{IF}$  and  $D_{VF}$  are the diffusion prefactors for each dopant–defect pair.

In the following example, the diffusivity of boron–interstitial pairs ( $D_{BI}$ ) and the diffusivity of boron–vacancy pairs ( $D_{BV}$ ) will be multiplied by `BoronIntDiffFactor` and `BoronVacDiffFactor`, respectively:

```
term name= BoronIntDiffFactor add Silicon \
    eqn = "exp(0.042 * $Vti * 125 * Germanium / 5e22)" store
term name= BoronVacDiffFactor add Silicon \
    eqn= "exp(0.042 * $Vti * 25 * Germanium / 5e22)" store
```

To allow Sentaurus Process to use these terms, specify a term with the name `<dopant>DiffFactor` or `<dopant><defect>DiffFactor`.

Anisotropic (optionally stress-dependent) diffusivities can be specified using the diffusion prefactors as well.

## High-Concentration Effects on Dopant Diffusion

To model experimentally observed sharp increases in arsenic diffusion in silicon at high dopant concentrations, diffusivity coefficients must be modified. Dunham and Wu [29] proposed that interactions of vacancies with more than one dopant result in the enhancement of dopant–vacancy pair diffusivity by a factor:

$$j = -DD_F \nabla C \quad (393)$$

$$D_F = 1 + \left( \frac{C_A}{C_{ref}} \right)^{C_{pow}} \quad (394)$$

where  $C_{As}$  is the active concentration of arsenic, and  $C_{ref} \sim 2 \times 10^{20} \text{ cm}^{-3}$  and  $C_{pow} \sim 4$  for arsenic. The correction factor can be applied to all dopant–defect pairs as long as the parameters are supplied. The model can be switched on with the command:

```
pdbSet <material> <dopant> <defect> HighConcDiffEffect 1
```

The default of the model is off (0). The model parameters are set using the command:

```
pdbSet <material> <dopant> <defect> Cref {<n>}
pdbSet <material> <dopant> <defect> Cpow {<n>}
```

For example:

```
pdbSet Silicon Arsenic Vacancy Cref 1.6e20
pdbSet Silicon Arsenic Vacancy Cpow 4.0
```

## 4: Diffusion

### Dopant Activation and Clustering

---

## Hydrogen Effects on Dopant Diffusion

To model experimentally observed sharp increases in boron diffusion in oxide at the presence of hydrogen, diffusivity coefficients of boron must be modified. Chakravarthi *et al.* [30] proposed that the presence of hydrogen results in the enhancement of boron diffusivity by the following factor:

$$j = -DD_F \nabla C \quad (395)$$

$$D_F = 1 + \left( \frac{C_H}{C_{ref}} \right)^{C_{pow}} \quad (396)$$

where  $C_H$  is the active concentration of hydrogen, and  $C_{ref} \sim 1 \times 10^{15} \text{ cm}^{-3}$  and  $C_{pow} \sim 1$  for boron. If hydrogen is present in the structure, the enhancement factor for boron will be applied automatically.

The model parameters are set using the command:

```
pdbSet <material> Hydrogen <dopant> Cref {<n>}  
pdbSet <material> Hydrogen <dopant> Cpow {<n>}
```

For example:

```
pdbSet Oxide Hydrogen Boron Cref 1.6e20  
pdbSet Oxide Hydrogen Boron Cpow 4.0
```

The correction factor can be applied to other dopants if the dopant is given in the dopant list using the command:

```
pdbSet <material> Hydrogen Dopants <list>
```

where  $<\text{list}>$  is the list of dopants. For example:

```
pdbSet Oxide Hydrogen Dopants "Boron Arsenic"
```

The diffusion of hydrogen itself is modeled using the constant diffusion model (see [Constant Diffusion Model on page 191](#)).

---

## Dopant Activation and Clustering

It is possible to select a different clustering or activation model for each dopant in different materials with the command:

```
pdbSet <material> <dopant> ActiveModel <model>
```

where `<dopant>` is a valid dopant name and `<model>` is one of the valid active models (`None`, `Solid`, `Transient`, `Cluster`, `ChargedCluster`, `BIC`, `FVCluster`, `Precipitation`, `FullPrecipitation`, or `Equilibrium`).

**NOTE** `BIC` is valid only for boron and is not recommended because the `ChargedCluster` model is better suited for modeling boron-interstitial clusters. `FVCluster` is valid only for fluorine. `FullPrecipitation` is valid only for copper.

## Dopant Active Model: None

If `ActiveModel` is set to `None`, all dopants are assumed to be active. No solid solubility or dopant clustering effects will be taken into account for dopant activation.

## Dopant Active Model: Solid

If `ActiveModel` is set to `Solid`, a simple solid solubility for the dopant activation is considered:

$$C_A^+ = \frac{C_A^{ss} C_A}{(C_A^{ss} + C_A)} \quad (397)$$

$C_A^{ss}$  is calculated by:

$$C_A^{ss} = f \cdot C_A^{ss0} \quad (398)$$

where  $f$  is the multiplication factor that is defined by:

```
pdbSet <material> <dopant> SS.Factor <expression>
```

and the solid solubility  $C_A^{ss0}$  of the dopant  $A$  that can be set with:

```
pdbSet <material> <dopant> Solubility {<n>}
```

when `SS.Model` is set to `Analytic`. However, when `SS.Model` is set to `Table`, the solid solubility is taken from the temperature-versus-solid solubility table.

The `SS.Model` is defined by:

```
pdbSet <material> <dopant> SS.Model <Analytic or Table>
```

## 4: Diffusion

### Dopant Activation and Clustering

The temperature-versus-solid solubility table is defined by:

```
pdbSet <material> <dopant> SS.Table <temp1 ss1 temp2 ss2 ... temp# ss#>
```

With the table, the solid solubility for the given temperature is logarithmically interpolated or extrapolated when the given temperature is out of range.

---

## Dopant Active Model: Precipitation

Setting ActiveModel to Precipitation or setting ActiveModel to the other activation model the list of More.Active.Model.List including Precipitation solves the transient equation:

$$\frac{\partial C_{App_t}}{\partial t} = -\frac{C_{App_t} - C_{App_t}^*}{\tau_{App_t}} \quad (399)$$

with the constraint:

$$0.0 \leq C_{App_t} \leq \max(C_A - \sum nC_{ACl} - C_{Amin}^+, 0.0) \quad (400)$$

$C_{App_t}$  is the precipitates concentration of the dopant and  $C_{App_t}^*$  is the equilibrium precipitates concentration given by:

$$C_{App_t}^* = C_A - \sum nC_{ACl} - C_{AEq} \quad (401)$$

where:

- $C_A$  is the total chemical concentration.
- $\sum nC_{ACl}$  represents the total dopant concentration in other clusters than precipitates.
- $C_{AEq}$  is the equilibrium active concentration calculated by [Dopant Active Model: Equilibrium on page 293](#). You do not have to switch on the Equilibrium model for the  $C_{AEq}$  calculation.

$\sum nC_{ACl}$  in [Eq. 400](#) and [Eq. 401](#) are included only when the other clustering model is invoked with the list of More.Active.Model.List, for example:

```
pdbSet Si Boron More.Active.Model.List { Precipitation }
pdbSet Si Boron ActiveModel Transient
```

The time constant  $\tau_{App_t}$  is given by:

$$\tau_{App_t} = \text{ClusteringTime for } C_{App_t} \leq C_{App_t}^* \quad (402)$$

$$\tau_{App_t} = \text{DeclusteringTime} \text{ for } C_{App_t} > C_{App_t}^* \quad (403)$$

The solution for  $C_{App_t}$  is named with `<species name>Ppts`; for example, `BPpts` for boron precipitates. The parameters `ClusteringTime` and `DeclusteringTime` are defined for the precipitates in the material, for example:

```
pdbSet Silicon BPpts ClusteringTime {[Arr 8e-16 -4.2]}
pdbSet Silicon BPpts DeclusteringTime {[Arr 8e-16 -4.2]}
```

$C_{Amin}^+$  is the minimum active concentration defined by the parameter `MinimumActive`, for example:

```
pdbSetString Silicon Boron MinimumActive "0.0"
```

## Initializing Precipitation Model

The initialization of the precipitation concentration depends on the value of the parameters `AmInit` and `AcInit`. The initial level of active concentration in amorphized and crystalline regions can be specified per dopant as `AmInit` and `AcInit`, respectively. You can specify the `AmInit` and `AcInit` parameters using:

```
pdbSet <material> <dopant> AcInit {<n>}
pdbSet <material> <dopant> AmInit {<n>}
```

If the `AcInit` parameter is not defined, the solid solubility of the dopant is used to calculate the `AcInit` parameter. If you want `AcInit` and `AmInit` to be a function of other fields for a specific dopant, define the terms `<dopant>AcInit` and `<dopant>AmInit` in your input files.

The precipitation model can be used with other activation models, for example:

```
pdbSet Si B ActiveModel BIC
pdbSet Si B More.Active.Model.List { Precipitation }
```

**NOTE** The items allowed in `More.Active.Model.List` are `Precipitation` or `ComplexCluster`. The equilibrium activation model cannot be used with the precipitation model.

When the precipitation model is invoked with other activation models, the initial concentrations of the clusters and the precipitates are set as follows.

In the amorphous region:

$$C_{App_t} = f_{App_t} \cdot \max(C_A - \text{AmInit}, 0.0) \quad (404)$$

$$C_{Aclust,i} = f_{Aclust,i} \cdot \max(C_A - \text{AmInit}, 0.0) \quad (405)$$

## 4: Diffusion

### Dopant Activation and Clustering

where the fraction ratio  $f_{App_t}$  for precipitation and  $f_{Aclust,i}$  for the cluster of other activation model  $i$  are written as:

$$f_{App_t} = \frac{\text{FractionAmor}_{ppt}}{\text{FractionAmor}_{ppt} + \text{FractionAmor}_{dopant} + \sum_i \text{FractionAmor}_i} \quad (406)$$

$$f_{Aclust,i} = \frac{\text{FractionAmor}_i}{\text{FractionAmor}_{ppt} + \text{FractionAmor}_{dopant} + \sum_i \text{FractionAmor}_i} \quad (407)$$

In the crystalline region:

$$\Delta C_{App_t} = f_{App_t} \cdot \max(C_{Aimplant} - \text{ACInit}, 0.0) \quad (408)$$

$$\Delta C_{Aclust,i} = f_{Aclust,i} \cdot \max(C_{Aimplant} - \text{ACInit}, 0.0) \quad (409)$$

where:

$$f_{App_t} = \frac{\text{FractionCryst}_{ppt}}{\text{FractionCryst}_{ppt} + \text{FractionCryst}_{dopant} + \sum_i \text{FractionCryst}_i} \quad (410)$$

$$f_{Aclust,i} = \frac{\text{FractionCryst}_i}{\text{FractionCryst}_{ppt} + \text{FractionCryst}_{dopant} + \sum_i \text{FractionCryst}_i} \quad (411)$$

The parameters `FractionAmor` and `FractionCryst` for the precipitation are written as:

```
pdbSet <material> <precipitates> FractionAmor <number>
pdbSet <material> <precipitates> FractionCryst <number>
```

## Dopant Active Model: FullPrecipitation

If you set `ActiveModel` to `FullPrecipitation` or set `ActiveModel` to another activation model in the `More.Active.Model.List` that includes `FullPrecipitation`, the selected model solves the reaction equations:



where  $C_{A_n}$  and  $C_{A_{n+1}}$  are the dopant clusters consisting of  $n$  and  $n + 1$  dopant atoms.

The reactions can be written as:

$$\begin{aligned} R_1 &\equiv k_{f_{n-1}} C_{A_{n-1}} - k_{r_n} C_{A_n} \\ R_2 &\equiv -(k_{f_n} C_{A_n} - k_{r_{n+1}} C_{A_{n+1}}) \end{aligned} \quad (413)$$

and the model is given by:

$$\frac{\partial C_{A_n}}{\partial t} = R_1 + R_2 \quad 2 \leq n < n_{\max} \quad (414)$$

where  $C_{A_n}$  is the density of clusters containing  $n$  atoms, and  $n_{\max}$  can be set using the command:

```
pdbSet Silicon Copper CL.Size {<n>}
```

The emission rate  $k_{r_n}$  is given by:

$$k_{r_n} = D_{\text{eff}} C_A^{\text{ss}} \frac{p}{n_i} \frac{A_{n-1}}{R_{\text{eff}} + K_{\text{ref}} \frac{p}{n_i}} e^{\left(\frac{+E_{fn}}{kT}\right)} \quad (415)$$

where:

- $D_{\text{eff}}$  is the effective diffusivity of the dopant.
- $C_A^{\text{ss}}$  is the solid solubility of the dopant.
- $\frac{A_{n-1}}{R_{\text{eff}}}$  is the capture efficiency of the dopant.
- $E_{fn}$  is its formation energy.
- $K_{\text{ref}}$  is the reference rate, which can be set by:

```
pdbSet <material> <dopant> Kref {<n>}
```

The formation energy is given as:

$$\begin{aligned} E_{fn} &= -(\Delta G_n^{\text{exc}} - \Delta G_{n-1}^{\text{exc}}) \\ \Delta G_n^{\text{exc}} &= 2\pi R_n \gamma \end{aligned} \quad (416)$$

where  $\gamma$  (eV/cm) is the surface/strain energy per unit perimeter, and  $R_n$  is the radius of the disk and is given as:

$$R_n = \sqrt{\frac{n\Omega}{\pi d}} \quad (417)$$

where  $\Omega$  is the volume density, and  $d$  is the thickness of the disk.

## 4: Diffusion

### Dopant Activation and Clustering

In addition:

$$A_n = 4\pi^2 R_n b \quad (418)$$

where  $b$  is the reaction distance.

The capture rate  $k_{f_n}$  is:

$$k_{f_n} = D_{\text{eff}} C_A^+ \frac{A_n}{R_{\text{eff}} + K_{\text{ref}} \frac{p}{n_i}} \quad (419)$$

where  $C_A^+$  is the active concentration of dopants, and  $A_n/R_{\text{eff}}$  and  $E_{fn}$  can be defined using the command:

```
pdbSet <material> <dopant> Bind.Cluster <cluster> {<n>}
```

where <cluster> is a valid cluster name (for example, Cu2, Cu3, or Cu21), and <n> must be an Arrhenius expression with a prefactor of  $A_n/R_{\text{eff}}$  and an activation energy of  $E_{fn}$ .

The following example sets  $A_n/R_{\text{eff}}$  to  $3.82578 \times 10^{-7}$  eV and  $E_{fn}$  to  $-1.29$  eV for  $n = 6$ :

```
pdbSet Silicon Copper Bind.Cluster Cu6 {[Arrhenius 3.82578e-07 -1.29]}
```

To modify the capture and emission rates,  $k_{f_n}$  and  $k_{r_n}$ , by complex prefactors, you can define the following terms in the command file:

```
term name= Cu2FormCopperFactor silicon add eqn= {equation} store  
term name= Cu2DissCopperFactor silicon add eqn= {equation} store
```

To reduce the number of equations and to increase time efficiency, it is assumed that small clusters fold to precipitates as:

$$\frac{\partial C_{A_{n_{\max}}}}{\partial t} = \frac{\partial C_{A_{\text{ppts}}}}{\partial t} = n_{\max} k_{f_{n-1}} C_{A_{n-1}} \quad (420)$$

## Initializing FullPrecipitation Model

The initial concentration of clusters and precipitates is set in the `diffPreProcess` procedure (see [Ion Implantation to Diffusion on page 339](#)). By default, there are no changes to clusters and precipitates in amorphous regions.

---

## Dopant Active Model: Transient

If `ActiveModel` is set to `Transient`, a transient dopant-cluster model is used. The transient dopant cluster is more complicated than the simple, solid solubility model. The following set of equations is solved along with the appropriate diffusion model equations:

$$\frac{\partial C_{AC}}{\partial t} = k_f \left( \frac{n}{n_i} \right)^{k_c} \left( \frac{1}{1 \times 10^{18}} \right)^{k_c - 1 + l_c} n_i^{k_c} \left( K_{Ffwd} (C_A^+)^{l_c} - K_{Fbwd} k_b (n_{ss})^{z l_c} n_i^{-z l_c} C_{AC} \left( \frac{n}{n_i} \right)^{-z l_c} \right) \quad (421)$$

where:

- $k_f$  is the forward-clustering reaction rate.
- $k_b$  is the de-clustering rate.
- $C_A^+$  is the active dopant concentration.
- $C_{AC}$  is the concentration of clusters.
- $l_c$  is the number of dopant atoms in the cluster.
- $k_c$  is the number of electrons participating in the reaction.
- $n$  is the electron concentration.
- $n_i$  is the intrinsic electron concentration.
- $n_{ss}$  is the electron concentration assuming that the dopant  $A$  reached the limits of solid solubility.

These quantities can be set using the commands:

```
pdbSet <material> <dopant> Kc      <n>
pdbSet <material> <dopant> Lc      <n>
pdbSet <material> <dopant> KcEqu    <n>
pdbSet <material> <dopant> CluRate <n>
```

where `KcEqu` and `CluRate` correspond to  $k_b$  and  $k_f$ . Initialization of transient dopant clusters is explained in [Ion Implantation to Diffusion on page 339](#). The default value of `KcEqu` is calculated by using:

$$K_{cEqu} = l_c \left( \frac{C_{ss}^{l_c}}{C_{sstot} - C_{ss}} \right) \quad (422)$$

where  $C_{ss}$  is the solid solubility of the unpaired dopant, set by the parameter `Solubility`, and  $C_{sstot}$  is the solid solubility of the total concentration of the dopant, set by the parameter `TotSolubility`, that is, the total dopant concentration at which the equilibrium active concentration of the dopant equals its solubility.

## 4: Diffusion

### Dopant Activation and Clustering

$K_{cEqu}$  can be set directly using the command:

```
pdbSet Silicon Arsenic KcEqu 1e66
```

or can be set indirectly using the commands:

```
pdbSet Silicon Arsenic Solubility 1e20
pdbSet Silicon Arsenic TotSolubility 1e21
```

and its modifying factors:

```
pdbSet Silicon Arsenic SS.Factor 1
pdbSet Silicon Arsenic Total.SS.Factor 1
```

In the case of alloys (for example, SiGe) where the mole-fraction interpolation scheme is switched on,  $K_{cEqu}$  is interpolated according to the mole fraction. By default, for example in SiGe, the above expression in [Eq. 422](#) is evaluated first for pure Si and pure Ge, and then is interpolated for the appropriate mole fraction. If the `KcEqu.From.Default.Formula` parameter is set to 1,  $K_{cEqu}$  is calculated from the same formula in [Eq. 422](#), but the mole-fraction interpolation is applied to individual parameters such as `Solubility` and `TotSolubility`, before the complete expression is evaluated. In such a situation, a direct setting of the parameter `KcEqu` is not applied. For example, this option is selected for phosphorus in Si using the following command:

```
pdbSet Silicon P KcEqu.From.Default.Formula 1
```

In addition,  $K_{Ffwd}$  and  $K_{Fbwd}$  are forward and backward reaction factors, respectively, and can be defined as:

```
term name= <dopant>TClusterForwardFac <mater> eqn= {user-defined equation}
      store
term name= <dopant>TClusterBackwardFac <mater> eqn= {user-defined equation}
      store
```

If they are not defined, their default value is 1.

Table 24 Solution names for transient model

Symbol	Boron	Arsenic	Phosphorus	Antimony	Indium
$C_{AC}$	B4	As3	P3	Sb3	In3

## Initializing Transient Model

If you switch on the transient dopant cluster model or cluster model, initialization of the dopant clusters is performed in the `diffPreProcess` procedure (see [Ion Implantation to Diffusion on page 339](#)).

The initialization of the dopant-cluster concentration depends on the value of the parameters `AmInit` and `AcInit`. The initial level of active concentration in amorphized and crystalline regions can be specified per dopant as `AmInit` and `AcInit`, respectively.

You can specify the `AmInit` and `AcInit` parameters using:

```
pdbSet <material> <dopant> AcInit <n>
pdbSet <material> <dopant> AmInit <n>
```

If the `AcInit` parameter is not defined, the solid solubility of the dopant is used to calculate the `AcInit` parameter. If you want `AcInit` and `AmInit` to be a function of other fields for a specific dopant, define the terms `<dopant>AcInit` and `<dopant>AmInit` in your input files.

For example:

```
term name= ArsenicAcInit silicon add \
      eqn= "Germanium/5e22 * [pdbDelayDouble Silicon Arsenic Solubility]" store
term name= ArsenicAmInit silicon add eqn= "Germanium/5e22*1e19" store
```

In this case `AcInit` and `AmInit` for arsenic are replaced with `ArsenicAcInit` and `ArsenicAmInit`.

If the dopant concentration is lower than `AcInit` in crystalline regions, dopants are considered to be active. If the dopant concentration is higher than `AcInit`, the number of active dopants is initially `AcInit`, and the concentration of clustered dopants is given by `Dopant - AcInit`. The following outlines the initialization of dopant clusters.

In crystalline regions:

$$\begin{aligned} \text{Dopant} &= \text{Dopant} + \min(\text{AcInit}, \text{Dopant\_Implant}) \\ \text{DopantCluster} &= \text{DopantCluster} + \text{Dopant\_Implant} - \min(\text{AcInit}, \text{Dopant\_Implant}) \end{aligned} \quad (423)$$

In amorphous regions:

$$\begin{aligned} \text{Dopant} &= \min(\text{AmInit}, \text{Dopant} + \text{DopantCluster} + \text{Dopant\_Implant}) \\ \text{DopantCluster} &= \text{Dopant} + \text{DopantCluster} + \text{Dopant\_Implant} \\ &\quad - \min(\text{AmInit}, \text{Dopant} + \text{DopantCluster} + \text{Dopant\_Implant}) \end{aligned} \quad (424)$$

where `Dopant` is the dopant name (for example, `Boron`, `B4`, and `Boron_Implant`). Smoothing also can be applied to dopant profiles using the `AmorpGamma` parameter (see [Ion Implantation to Diffusion on page 339](#)).

## 4: Diffusion

### Dopant Activation and Clustering

---

## Dopant Active Model: Cluster

If `ActiveModel` is set to `Cluster`, a dopant–defect cluster model is used. The model is primarily implemented to simulate arsenic–vacancy clusters, but if the model parameters are provided, it is possible to simulate other dopant–defect clusters.

The model assumes that arsenic–vacancy clusters are formed in silicon during arsenic deactivation [31][32]. It is also assumed that neutral clusters ( $As_m V_k$ ) are formed. Different charge states are taken into account by:



$$f = (m - kj)e, \text{ if } (kj - m) < 0 \quad (426)$$

$$f = (m - kj)h, \text{ if } (kj - m) \geq 0 \quad (427)$$

where  $j$  denotes interstitial charge,  $e$  and  $h$  are the electron and hole densities, and  $m$  and  $k$  are the dopant and defect sizes, respectively.

The following commands can be used to set the reacting defect species,  $m$  and  $k$ , respectively:

```
pdbSet <material> <dopant> ClusterDefects <c>
pdbSet <material> <dopant> <defect> ClusterSizes {{<n> <n>}}
```

for example:

```
pdbSet Silicon Arsenic ClusterDefects Vac
pdbSet Silicon Arsenic Vacancy ClusterSizes {{4 1}}
```

where 4 is the number of arsenic atoms in the cluster and 1 is the number of vacancies in the cluster. They form the  $As_4 Vacancy$  clusters.

**NOTE** Cluster sizes are defined as { $i$   $j$ } where  $i$  and  $j$  are integers, and are separated by a space.

The reaction rate for the cluster formation can be written as:

$$R_j \equiv K_{fj} C_{As}^m \left( \frac{n}{n_i} \right)^{m-kj} - K_{rj} C_{As_m V_k} C_I^0 \left( \frac{n}{n_i} \right)^{kj} \quad (428)$$

where  $C_{As}$  is the active arsenic concentration,  $C_{As_m V_k}$  is the arsenic–vacancy cluster concentration,  $C_I^0$  is the neutral interstitial concentration,  $n$  is the electron concentration,  $n_i$  is the intrinsic electron concentration,  $K_{fj}$  is the forward reaction rate, and  $K_{rj}$  is the backward reaction rate.

An additional assumption was made for all  $j$ :

$$\frac{K_{rj}}{K_{fj}} = K_{equ} \quad (429)$$

Then, the total rate  $R$  is the sum of  $R_j$  over all  $j$ :

$$R = \sum_i K_{fj} \left( \frac{n}{n_i} \right)^{kj} \left( C_{As}^m \left( \frac{n}{n_i} \right) - K_{equ} C_{As_m} V_k C_I^0 \right) \quad (430)$$

The forward reaction rate  $K_{fj}$  can be set using the command:

```
pdbSet <material> <dopant> <defect> CluRateChargeStates {<n>}
```

for example:

```
pdbSet Silicon Arsenic Vacancy CluRateChargeStates
{-2 {[Arrhenius 5.0e-42 7.8]}}
{-1 {[Arrhenius 5.0e-42 7.8]}}
{0 {[Arrhenius 5.0e-42 7.8]}}
{1 {[Arrhenius 5.0e-42 7.8]}}
{2 {[Arrhenius 5.0e-42 7.8]}}
```

The equilibrium reaction rate is calculated by:

$$K_{equ} = \frac{K_{cEqu} \left( \frac{n_{ss}}{n_i} \right)^m}{(C_I^*)^k} \quad (431)$$

where  $n_{ss}$  is the electron concentration assuming that arsenic reached the limits of solid solubility and  $C_I^*$  is the equilibrium concentration of interstitials.  $K_{cEqu}$  is given as:

$$K_{cEqu} = m \left( \frac{C_{ss}^m}{C_{sstot} - C_{ss}} \right) \quad (432)$$

where  $C_{ss}$  is the solid solubility of the unpaired arsenic dopants and  $C_{sstot}$  is the solid solubility of total arsenic concentration.

You can either set the solid solubility values or  $K_{cEqu}$  using the commands:

```
pdbSet Silicon Arsenic Solubility 1e20
pdbSet Silicon Arsenic TotSolubility 1e21
pdbSet Silicon Arsenic Vac KcEqu 1e66
```

## 4: Diffusion

### Dopant Activation and Clustering

In addition, Solubility and TotSolubility can be changed through their modifying factors:

```
pdbSet Silicon Arsenic SS.Factor 1  
pdbSet Silicon Arsenic Total.SS.Factor 1
```

**NOTE** For high-concentration effects, see [High-Concentration Effects on Dopant Diffusion on page 275](#). For smoothing dopant profiles around amorphous to crystalline regions, see [Ion Implantation to Diffusion on page 339](#).

Table 25 Solution for cluster model

Symbol	Arsenic
$C_{As_m V_k}$	As4Vac

## Initializing Cluster Model

Initially, dopant-interstitial cluster concentrations (for example, As4Vac) are set to zero. If there is an existing cluster concentration field, the field is used. If there are amorphized regions, dopant-defect pairs and clusters are redistributed in these regions (see [Initializing Dopant and Dopant-Defect Clusters on page 302](#)). In addition, you can initialize any of the cluster concentration fields using the select command in the command file.

---

## Dopant Active Model: NeutralCluster

The NeutralCluster model assumes that all reactants as well as clusters are neutral. If the NeutralCluster model is selected, the following reactions are taken into account:



where  $i, j$  are the number of dopant and defect atoms in the cluster, respectively. The clusters can be specified using the command:

```
pdbSet <material> <dopant> <defect> ClusterSizes <list>
```

For example, the carbon clusters are defined by:

```
pdbSet Silicon Carbon Interstitial ClusterSizes {{1 0} {1 1} {2 0} {2 1} {3 1}}
```

**NOTE** This sets up the diffusion equations for  $C$ ,  $CI$ ,  $C_2$ ,  $C_2I$ , and  $C_3I$ . Cluster sizes given in the ClusterSizes list increase in size. For example, the following is incorrect:

```
pdbSet Si Boron Int ClusterSizes { {1 0} {3 1} {1 1} }
```

**NOTE** If you add new cluster sizes, you must define the aliases for the new clusters, for example:

```
alias C2I2 Carbon2Int2
```

The reactions are written as:

$$R_{IAI} \equiv K_{fIA_iI_j}(C_{A_iI_j}C_I - B_{IA_iI_j}C_{A_iI_{j+1}}) \quad (439)$$

$$R_{VAI} \equiv K_{fVA_iI_j}(C_{A_iI_j}C_V - B_{VA_iI_j}C_{A_iI_{j-1}}) \quad (440)$$

$$R_{AI} \equiv K_{fAIA_iI_j}(C_{A_iI_j}C_{AI} - B_{AIA_iI_j}C_{A_{i+1}I_{j+1}}) \quad (441)$$

$$R_{VAV} \equiv K_{fVA_iV_j}(C_{A_iV_j}C_V - B_{VA_iV_j}C_{A_iV_{j+1}}) \quad (442)$$

$$R_{IAV} \equiv K_{fIA_iV_j}(C_{A_iV_j}C_I - B_{IA_iV_j}C_{A_iV_{j-1}}) \quad (443)$$

$$R_{AV} \equiv K_{fAVA_iV_j}(C_{A_iV_j}C_{AV} - B_{AVA_iV_j}C_{A_{i+1}V_{j+1}}) \quad (444)$$

where:

- $K_{fIA_iI_j}$ ,  $K_{fVA_iI_j}$ ,  $K_{fAIA_iI_j}$ ,  $K_{fVA_iV_j}$ ,  $K_{fIA_iV_j}$ , and  $K_{fAVA_iV_j}$  are the forward reaction rates.
- $B_{IA_iI_j}$ ,  $B_{VA_iI_j}$ ,  $B_{AIA_iI_j}$ ,  $B_{VA_iV_j}$ ,  $B_{IA_iV_j}$ , and  $B_{AVA_iV_j}$  are the binding coefficients.

## 4: Diffusion

### Dopant Activation and Clustering

To set these parameters, use the following commands:

```
pdbSet <material> <dopant> Interstitial KfCluster    <cluster> {<n>}
pdbSet <material> <dopant> Vacancy      KfCluster    <cluster> {<n>}
pdbSet <material> <dopant> <pair>       KfCluster    <cluster> {<n>}
pdbSet <material> <dopant> Interstitial Bind.Cluster <cluster> {<n>}
pdbSet <material> <dopant> Vacancy      Bind.Cluster <cluster> {<n>}
pdbSet <material> <dopant> <pair>       Bind.Cluster <cluster> {<n>}
```

where `<cluster>` is a valid cluster name (for example, `C2`, `C2I`, `C3I`, `C3I2`), and `<pair>` is a dopant–interstitial pair (for example, `CarbonInt`) or a dopant–vacancy pair.

The following example sets the forward reaction rate of the `CarbonInt` and `C3I2` reaction to `{ [Arrhenius 1e-10 0.3] }`:

```
pdbSet Silicon Carbon CarbonInt KfCluster C3I2 { [Arrhenius 1e-10 0.3] }
```

## Initializing NeutralCluster Model

Initially, cluster concentrations are set to zero. If there is an existing cluster concentration field, the field is used. If there are amorphized regions, dopant–defect pairs and clusters are redistributed in these regions (see [Initializing Dopant and Dopant–Defect Clusters on page 302](#)).

In addition, you can initialize any of the cluster concentration fields using the `select` command in the command file.

## Carbon Cluster

The carbon-clustering model uses the `NeutralCluster` model. The following solutions are solved for the carbon model.

Table 26 Solution names for carbon model

Symbol	Solution name	Symbol	Solution name
$C$	Carbon	$C_3I_2$	C3I2
$CI$	CarbonInt	$C_4I_2$	C4I2
$C_2$	C2	$C_4I_3$	C4I3
$C_{2I}$	C2I	$C_5I_3$	C5I3
$C_3I$	C3I	$C_5I_4$	C5I4

## Nitrogen Cluster

The nitrogen-clustering model uses the `NeutralCluster` model. The following solutions are solved for the nitrogen model.

Table 27 Solution names for nitrogen model

Symbol	Solution name
<i>N</i>	Nitrogen
<i>NI</i>	NitrogenInt
<i>NV</i>	NV
<i>N<sub>2</sub></i>	NDimer
<i>N<sub>2</sub>V</i>	N2V
<i>N<sub>2</sub>V<sub>2</sub></i>	N2V2

`NDimer` is a cluster; therefore, it is initialized by `FractionAmor` or `FractionCryst` or both in the same way as other cluster initializations.

**NOTE** If an activation model other than `NeutralCluster` is used for nitrogen, the reactions between `Nitrogen` and `NDimer` are switched off.

`NV` is not a mobile pair but an immobile cluster. For example, the reaction is defined by:

```

pdbSet Si N Vac ClusterSizes { {1 0} {1 1} }
pdbSet Si N Vac KfCluster N {[expr [DiffLimit Silicon Vac 0.0]]}
pdbSet Si N Vac Bind.Cluster N {[Arr 5e22 1.58]}

```

## Dopant Active Model: FVCluster

If `ActiveModel` is set to `FVCluster`, the fluorine–vacancy cluster model is used. The model based on fluorine–point defect interaction is implemented [33]. The primary reactions used in the model are:



where *F* is mobile fluorine, *I* is interstitial, *V* is vacancy, and  $F_3V$  is an immobile cluster (three fluorine atoms bound to a vacancy). The model assumes that  $F_3V$  is the dominant cluster.

## 4: Diffusion

### Dopant Activation and Clustering

These reactions can be written as:

$$R_1 \equiv K_I D_{I0} \left( C_{F_3V} C_I - \frac{C_F^3}{C_{F_3V}^*} \right) \quad (447)$$

$$R_2 \equiv K_V D_{I0} \left( C_{F_3V} - \frac{C_F^3 C_V}{C_{F_3V}^* C_I^* C_V^*} \right) \quad (448)$$

where  $K_I$  and  $K_V$  are the forward reaction rates. They can be defined using the commands:

```
pdbSet <material> Fluorine F3V KfI {<n>}
pdbSet <material> Fluorine F3V KfV {<n>}
```

$D_{I0}$  is the diffusivity of neutral interstitials,  $C_{F_3V}$  is the concentration of fluorine–vacancy clusters,  $C_F$  is the concentration of fluorine, and  $C_I$  and  $C_V$  are the concentration of interstitials and vacancies, respectively.

Quantities with a superscript (\*) correspond to their equilibrium values. The equilibrium value of  $C_{F_3V}$  can be set by:

```
pdbSet <material> Fluorine F3V Cstar <n>
```

The differential equations that describe the model are:

$$\frac{\partial C_F}{\partial t} = \nabla \bullet (D_0 \nabla C_F) + 3R_1 + 3R_2 \quad (449)$$

$$\frac{\partial C_{F_3V}}{\partial t} = -R_1 - R_2 \quad (450)$$

The fluorine diffusion coefficient,  $D_0$ , can be set using the command:

```
pdbSet <material> Fluorine Dstar {<n>}
```

The quantity  $R_1$  is subtracted from  $R_I^{clus}$  and the quantity  $R_2$  is added to  $R_V^{clus}$ .

**NOTE** The fluorine model is switched off by default. To switch it on, use the following commands:

```
solution add name= Fluorine ifpresent= "Fluorine" !negative
solution add name= F3V ifpresent= "F3V Fluorine" !negative
```

Table 28 Solution names for fluorine model

Symbol	Solution name
$C_F$	Fluorine
$C_{F_3V}$	F3V

## Initializing the FVCluster Model

You can select a different initialization model for fluorine with the command:

```
pdbSet <material> Fluorine FVCluster.Init <model>
```

where <model> is either FV.Full or DAC.

If the FV.Full model is selected, it is assumed that the complete fluorine dose is implanted as fluorine–vacancy clusters ( $C_{F_3V}$ ). Since the ‘+1’ model is used to generate the excess interstitials, this effectively introduces interstitials of a concentration equal to  $C_{F_3V}$ , except in amorphous regions.

If the DAC model is selected, initially, the fluorine–vacancy cluster concentration is set to zero. If there is an existing cluster concentration field, this field is used. If there are amorphized regions, clusters are redistributed in these regions (see [Initializing Dopant and Dopant–Defect Clusters on page 302](#)). In addition, you can initialize any of the cluster concentration fields using the select command in the input command file.

**NOTE** The DAC model does not modify the vacancy field during initialization of F<sub>3</sub>V.

## Dopant Active Model: Equilibrium

If ActiveModel is set to Equilibrium, solid solubility or dopant clustering is considered. In the clustering model, the active concentration of the dopant,  $C_A^+$ , is obtained by solving:

$$C_{AS} = C_A^+ + (K_{CTN} C_A^+)^{K_{CTN,F}} \quad (451)$$

where  $K_{CTN}$  and  $K_{CTN,F}$  are clustering parameters and can be set by:

```
pdbSet <material> <dopant> Kctn {<n>}
pdbSet <material> <dopant> Kctn.F {<n>}
```

## 4: Diffusion

### Dopant Activation and Clustering

$C_{AS}$  is also given by:

$$C_{AS} = \begin{cases} C_A & C_A < 0.9C_A^{SS} \\ C_A^{SS} - \frac{(C_A - 1.1C_A^{SS})^2}{0.4C_A^{SS}} & 0.9C_A^{SS} \leq C_A \leq C_A^{SS} \\ C_A^{SS} & C_A > 1.1C_A^{SS} \end{cases} \quad (452)$$

where  $C_A$  is the total unpaired dopant concentration, and  $C_A^{SS}$  is calculated as described in [Dopant Active Model: Solid on page 277](#).

If the clustering parameters  $K_{CTN.F}$  and  $K_{CTN}$  are zero, the active concentration is determined by [Eq. 452](#); otherwise, [Eq. 451](#) is solved numerically.

Table 29 Solution names for equilibrium model

Symbol	Boron	Arsenic	Phosphorus	Antimony	Indium
$C_{AS}$	BoronEqu	ArsenicEqu	PhosphorusEqu	AntimonyEqu	IndiumEqu

When the parameter `Equil.Active.Conc` is specified, the expression of `Equil.Active.Conc` is evaluated for the active concentration in equilibrium, instead of calculating [Eq. 451](#) and [Eq. 452](#). For example:

```
pdbSet Si B Equil.Active.Conc "(Boron>1E19)?(1E19):(Boron)"
```

## Dopant Active Model: BIC

`ActiveModel` can be set to `BIC` for boron. The model is implemented to simulate boron-interstitial clusters (BICs).

The model makes no assumptions regarding the diffusion model to generate the diffusion equation for the substitutional and the mobile species. However, it should be used with either the `Pair` or `React` model. The model does not take charge-state-dependent reaction rates into account.

The following types of clustering reaction are taken into account:



where  $i, j$  are the number of boron and interstitial atoms in the cluster  $B_iI_j$ , respectively.

The clusters can be specified using the command:

```
pdbSet Silicon Boron Interstitial ClusterSizes <list>
```

The following example sets up the diffusion equations for  $BI_2$ ,  $B_2I$ ,  $B_3I$ , and  $B_3I_2$ :

```
pdbSet Silicon Boron Interstitial ClusterSizes {{1 0} {1 1} {1 2} {2 1} \
{3 1} {3 2}}
```

**NOTE** Cluster sizes given in the `ClusterSizes` list are increasing in size. For example, the following command is incorrect:

```
pdbSet Si B Int ClusterSizes { {1 0} {3 1} {1 1} }
```

The reactions are written as:

$$R_I \equiv K_{fIB_iI_j}(C_{B_iI_j}C_I - B_{IB_iI_j}C_{B_iI_{j+1}}) \quad (456)$$

$$R_V \equiv K_{fVB_iI_j}(C_{B_iI_j}C_V - B_{VB_iI_j}C_{B_iI_{j-1}}) \quad (457)$$

$$R_{CI} \equiv K_{fBI_{B_iI_j}}(C_{B_iI_j}C_{BI} - B_{BI_{B_iI_j}}C_{B_{i+1}I_{j+1}}) \quad (458)$$

where  $K_{fIB_iI_j}$ ,  $K_{fVB_iI_j}$ , and  $K_{fBI_{B_iI_j}}$  are the forward reaction rates, and  $B_{IB_iI_j}$ ,  $B_{VB_iI_j}$ , and  $B_{BI_{B_iI_j}}$  are the binding coefficients.

To set these parameters, the following commands can be used:

```
pdbSet <material> Boron Interstitial KfCluster <cluster> {<n>}
pdbSet <material> Boron Vacancy KfCluster <cluster> {<n>}
pdbSet <material> Boron BoronInt KfCluster <cluster> {<n>}
pdbSet <material> Boron Interstitial Bind.Cluster <cluster> {<n>}
pdbSet <material> Boron Vacancy Bind.Cluster <cluster> {<n>}
pdbSet <material> Boron BoronInt Bind.Cluster <cluster> {<n>}
```

where `<cluster>` is a valid cluster name, for example, `BI2`, `B2I`, `B3I`, `B3I2`.

The following example sets the forward reaction rate of the `BoronInt` and `B3I2` reaction to `{ [Arrhenius 1e-10 0.3] }`:

```
pdbSet Silicon Boron BoronInt KfCluster B3I2 { [Arrhenius 1e-10 0.3] }
```

The differential equations for the clusters are:

$$\frac{\partial}{\partial t} B_{iI_j} = -R_I - R_V - R_{BI} \quad (459)$$

## 4: Diffusion

### Dopant Activation and Clustering

The reactions  $R_I$ ,  $R_V$ , and  $R_{BI}$  are added to the appropriate point-defect equations, and substitutional and mobile boron diffusion equations.

Table 30 Solution names for BIC model

Symbol	Solution name
$C_B$	Boron
$C_{BI}$	BoronInt
$C_{BI_2}$	BI2
$C_{B_2I}$	B2I
$C_{B_3I}$	B3I
$C_{B_3I_2}$	B3I2

## Initializing BIC Model

Initially, boron-interstitial cluster concentrations (for example, B3I) are set to zero. If there is an existing cluster concentration field, the field is used. If there are amorphized regions, boron defect pairs, and clusters are redistributed in these regions. For details, see [Initializing Dopant and Dopant–Defect Clusters on page 302](#). In addition, you can initialize any of the cluster concentrations field using the `select` command in the input command file.

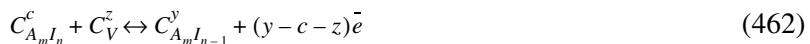
---

## Dopant Active Model: ChargedCluster

`ActiveModel` can be set to `ChargedCluster` for dopant. The model is implemented to simulate dopant-defect clusters including different charge states.

The model makes no assumptions regarding the diffusion model to generate the diffusion equation for the substitutional and the mobile species. However, it should be used with either the `Pair` or `ChargedPair` or `React` or `ChargedReact` model.

The following types of clustering reaction are taken into account:





where:

- $m, n$  are the number of dopant and interstitial atoms in the cluster  $C_{A_m I_n}$ , respectively, and they are the number of dopant and vacancy atoms in the cluster  $C_{A_m V_n}$ , respectively.
- $C_I, C_V$  are the concentration of interstitials and vacancies.
- $c, y, z$  are different charge states of clusters and point defects.

The clusters can be specified using the command:

```
pdbSet Silicon <dopant> <defect> ClusterSizes <list>
```

The following example sets up the diffusion equations for  $BI_2$ ,  $B_2I$ ,  $B_3I$ , and  $B_3I_2$ :

```
pdbSet Silicon Boron Interstitial ClusterSizes {{1 0} {1 1} {1 2} {2 1} \
{3 1} {3 2}}
```

**NOTE** Cluster sizes given in the ClusterSizes list are increasing in size. For example, the following command is incorrect:

```
pdbSet Si Boron Int ClusterSizes { {1 0} {3 1} {1 1} }
```

The reactions are written as:

$$R_{A_m I_{n+1}} \equiv K_{fA_m I_{n+1}} \left( C_{A_m I_n}^c C_I^z - K_{rA_m I_{n+1}} C_{A_{m+1} I_{n+1}}^y \left( \frac{n}{n_i} \right)^{(y-c-z)} \right) \quad (464)$$

$$R_{A_{m+1} I_{n+1}} \equiv K_{fA_{m+1} I_{n+1}} \left( C_{A_m I_n}^c C_{AI}^z - K_{rA_{m+1} I_{n+1}} C_{A_{m+1} I_{n+1}}^y \left( \frac{n}{n_i} \right)^{(y-c-z)} \right) \quad (465)$$

$$R_{A_m I_{n-1}} \equiv K_{fA_m I_{n-1}} \left( C_{A_m I_n}^c C_V^z - K_{rA_m I_{n-1}} C_{A_{m+1} I_{n-1}}^y \left( \frac{n}{n_i} \right)^{(y-c-z)} \right) \quad (466)$$

$$R_{A_{m+1} I_{n-1}} \equiv K_{fA_{m+1} I_{n-1}} \left( C_{A_m I_n}^c C_{AV}^z - K_{rA_{m+1} I_{n-1}} C_{A_{m+1} I_{n-1}}^y \left( \frac{n}{n_i} \right)^{(y-c-z)} \right) \quad (467)$$

where:

- $K_{fA_m I_{n+1}}, K_{fA_{m+1} I_{n+1}}, K_{fA_m I_{n-1}},$  and  $K_{fA_{m+1} I_{n-1}}$  are the forward reaction rates.
- $K_{rA_m I_{n+1}}, K_{rA_{m+1} I_{n+1}}, K_{rA_m I_{n-1}},$  and  $K_{rA_{m+1} I_{n-1}}$  are the equilibrium constants.

## 4: Diffusion

### Dopant Activation and Clustering

The forward reaction rates are a function of the lattice spacing ( $L$ ), the capture radius factor ( $r$ ), and the diffusion of point defect ( $D_I^z, D_V^z$ ) or dopant-defect pair ( $D_{AI}^z, D_{AV}^z$ ):

$$K_{fA_mI_{n+1}} \propto 4\pi L r_{A_mI_{n+1}} D_I^z \quad (468)$$

$$K_{fA_{m+1}I_{n+1}} \propto 4\pi L r_{A_{m+1}I_{n+1}} D_{AI}^z \quad (469)$$

$$K_{fA_mI_{n-1}} \propto 4\pi L r_{A_mI_{n-1}} D_V^z \quad (470)$$

$$K_{fA_{m+1}I_{n-1}} \propto 4\pi L r_{A_{m+1}I_{n-1}} D_{AV}^z \quad (471)$$

To set the capture radius factor parameter, use the following command:

```
pdbSet <material> <dopant> <defect | mobile> CaptureRadiusFactor <cluster> \
{<expression>}
```

where `mobile` is the mobile species (for example, `BoronInt`, `BoronVac`). For example:

```
pdbSet Silicon Boron BoronInt CaptureRadiusFactor B2 1.3
```

means that the capture radius for  $B_2 + BoronInt \leftrightarrow B_3I$  is 1.3 times the lattice spacing.

The equilibrium conditions are calculated internally using:

$$C_{A_mI_n}^c = \frac{NC_A^m}{(5 \times 10^{22})^{m-1}} \frac{C_I}{C_I^0} \left(\frac{n}{n_i}\right)^{-m-c} e^{\frac{E_{form}}{kT}} \quad (472)$$

where  $N$  is the cluster degeneracy,  $c$  is the cluster charge, and  $E_{form}$  is the formation energy of the cluster.

To set these parameters, use the following commands:

```
pdbSet <material> <dopant> <defect> ClusterDegeneracy <cluster> {<n>}
pdbSet <material> <dopant> <defect> ClusterCharge <cluster> {<n>}
pdbSet <material> <dopant> <defect> ClusterFormE <cluster> {<expression>}
```

where `<cluster>` is a valid cluster name, for example, `B12`, `B2I`, `B3I`, or `B3I2`.

The following example sets the formation energy of cluster  $B_3I_2$  to 0.3 eV:

```
pdbSet Silicon Boron Int ClusterFormE B3I2 {0.3}
```

The differential equations for the clusters are:

$$\frac{\partial C_{A_m I_n}}{\partial t} = -R_{A_m I_{n+1}} - R_{A_{m+1} I_{n+1}} - R_{A_m I_{n-1}} - R_{A_{m+1} I_{n-1}} \quad (473)$$

The reactions are added to the appropriate point-defect equations, and substitutional and mobile boron diffusion equations.

Table 31 Solution names for ChargedCluster model  
assuming the base defect is boron

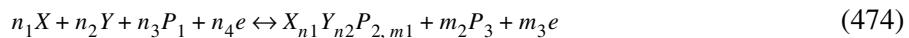
Symbol	Solution name
$C_B$	Boron
$C_{BI}$	BoronInt
$C_{BI_2}$	BI2
$C_{B_2I}$	B2I
$C_{B_3I}$	B3I
$C_{B_3I_2}$	B3I2

## Initializing ChargedCluster Model

Initially, dopant-interstitial cluster concentrations (for example, B3I) are set to zero. If there is an existing cluster concentration field, the field is used. If there are amorphized regions, dopant-defect pairs and clusters are redistributed in these regions (see [Initializing Dopant and Dopant-Defect Clusters on page 302](#)). In addition, you can initialize any of the cluster concentration fields using the `select` command in the command file.

## Dopant Active Model: ComplexCluster

The reaction of the ComplexCluster model is as follows:



where:

- $X$  and  $Y$  denote two different dopant species.
- $X_{n1} Y_{n2} P_{2,m1}$  is a complex cluster.
- $P_1$ ,  $P_2$ , and  $P_3$  denote point defects, that is, either a Si self-interstitial or vacancy.
- $e$  indicates an electron.

## 4: Diffusion

### Dopant Activation and Clustering

The reaction is formulated by:

$$R = K_f C_{norm} \left( \frac{C_{A_1}^+}{C_{norm}} \right)^{n_1} \left( \frac{C_{A_2}^+}{C_{norm}} \right)^{n_2} \left( \frac{P_1}{P_1^*} \right)^{n_3} \left( \frac{n}{n_i} \right)^{n_4} - K_r C_{X_{n1}Y_{n2}P_{2,m1}} \left( \frac{P_3}{P_3^*} \right)^{m_2} \left( \frac{n}{n_i} \right)^{m_3} \quad (475)$$

$C_{norm}$  is the normalization factor that is specified by:

```
term name= ${X_{n1}Y_{n2}P_{2,m1}}NormValue <material> add eqn= <equation> store
```

By default,  $C_{norm}$  is set to the intrinsic carrier concentration,  $n_i$ .

The chemical elements of the complex cluster  $X_{n1}Y_{n2}P_{2,m1}$  are defined by:

```
pdbSetDoubleArray <material> <X_{n1}Y_{n2}P_{2,m1}> Component.List \
{<X> <n1> <Y> <n2> <P2> <m1>}
```

For example:

```
pdbSetDoubleArray Silicon BCI Component.List { Boron 1 Carbon 1 Int 1 }
```

When the charge state of the complex cluster,  $P_3$ ,  $m_2$ , and  $m_3$  are given, the other unknowns  $P_1$ ,  $n_3$ , and  $n_4$  are determined automatically.

$P_3$ ,  $m_2$ , and  $m_3$  are specified by:

```
pdbSetDoubleArray <material> <X_{n1}Y_{n2}P_{2,m1}> Product.List \
{<P3> <m2> <Electron | Hole> <|m3|>}
```

For example:

```
pdbSetDoubleArray Silicon BCI Product.List { Electron 1 }
pdbSetDoubleArray Silicon BCI ChargeState { 0 1.0 }
```

With the two examples above, the reaction is defined as follows:

$$R = K_f n_i \left( \frac{C_B^+}{n_i} \right) \left( \frac{C_C^+}{n_i} \right) \left( \frac{I}{I^*} \right) - K_r C_{BCI} \left( \frac{n}{n_i} \right) \quad (476)$$

The forward and reverse reaction rates,  $K_f$  and  $K_r$ , are calculated by:

$$K_f = factor_f \times K_{f0} \quad (477)$$

$$K_r = factor_r \times K_{r0} \quad (478)$$

where  $K_f$ ,  $K_r$ ,  $factor_f$ , and  $factor_r$  are specified by:

```

pdbSetDouble <material> <Xn1Yn2P2,m1> KF <n>
pdbSetDouble <material> <Xn1Yn2P2,m1> KR <n>
term name= ${Xn1Yn2P2,m1}KFFactor <material> add eqn= <equation> store
term name= ${Xn1Yn2P2,m1}KRFactor <material> add eqn= <equation> store

```

By default,  $factor_f$  and  $factor_r$  are set to 1.0.

## Initializing ComplexCluster Model

The initialization of the clusters in the ComplexCluster model is performed in a similar way to that of the precipitation model (see [Initializing Precipitation Model on page 279](#)).

The ComplexCluster model can be used with other activation models, for example:

```

pdbSet Si B ActiveModel BIC
pdbSet Si B More.Active.Model.List { ComplexCluster }

```

**NOTE** The items allowed in More.Active.Model.List are Precipitation or ComplexCluster.

For the initialization of the clusters with the other activation models, see [Initializing Precipitation Model on page 279](#).

When the multiple dopant species are involved in the reaction of the ComplexCluster model, the initialization is more complicated because the dose conservations of both dopant species must be satisfied. For example, the silicon substrate is doped with  $1 \times 10^{20} \text{ cm}^{-3}$  boron atoms and  $1 \times 10^{20} \text{ cm}^{-3}$  carbon atoms, and the following specifications for their activation models and initializations are given by:

```

pdbSet Si B ActiveModel ComplexCluster
pdbSet Si C ActiveModel ComplexCluster
pdbSet Si B AmInit 4E19
pdbSetDouble Si C AmInit 1E19
pdbSet Si BCI FractionAmor 1.0

```

In the amorphous region, the initial boron active concentration needs to be set to  $4 \times 10^{19} \text{ cm}^{-3}$ . This means that the BCI concentration must be  $6 \times 10^{19} \text{ cm}^{-3}$ , while the initial active concentration of carbon is set to  $1 \times 10^{19} \text{ cm}^{-3}$ . Therefore, the BCI concentration is supposed to be set to  $9 \times 10^{19} \text{ cm}^{-3}$ . In this case, the smaller BCI concentration  $6 \times 10^{19} \text{ cm}^{-3}$  is set for BCI, so that the active concentration of carbon is adjusted to  $4 \times 10^{19} \text{ cm}^{-3}$ ; although, AmInit for carbon is given as  $1 \times 10^{19} \text{ cm}^{-3}$ .

## 4: Diffusion

### Dopant Activation and Clustering

---

## Initializing Dopant and Dopant–Defect Clusters

If you switch on the BIC, ChargedCluster, CarbonCluster, React, ChargedReact, or NeutralReact model, initialization of the dopant and dopant-defect clusters are performed in the diffPreProcess procedure (see [Ion Implantation to Diffusion on page 339](#)). It is possible to redistribute dopants and dopant-defect clusters in the amorphous and crystalline regions after implantation.

The initialization of the dopant and dopant-defect clusters depends on the value of the parameters `AmInit`, `AcInit`, `FractionCryst`, and `FractionAmor`. The initial level of active concentration of dopants in amorphized and crystalline regions can be specified per dopant as `AmInit` and `AcInit`, respectively. You can specify the `AmInit` and `AcInit` parameters by using:

```
pdbSet <material> <dopant> AcInit {<n>}  
pdbSet <material> <dopant> AmInit {<n>}
```

If the `AcInit` or `AmInit` parameter is not defined, the default value of  $5 \times 10^{22}$  is used. If you want `AcInit` and `AmInit` to be a function of other fields for a specific dopant, define the terms `<dopant>AcInit` and `<dopant>AmInit` in your input files.

For example:

```
term name= ArsenicAcInit silicon add \  
    eqn= "Germanium/5e22 * [pdbDelayDouble Silicon Arsenic Solubility]" store  
term name= ArsenicAmInit silicon add eqn= "Germanium/5e22*1e19" store
```

In this case, `AcInit` and `AmInit` for arsenic are replaced with `ArsenicAcInit` and `ArsenicAmInit`.

The `FractionCryst` and `FractionAmor` parameters are used to calculate the fraction of dopants and dopant-defect clusters in crystalline and amorphized regions. To specify the `FractionCryst` and `FractionAmor` parameters, use:

```
pdbSetDouble <material> <dopant | cluster> FractionCryst {<n>}  
pdbSetDouble <material> <dopant | cluster> FractionAmor {<n>}
```

The following outlines the initialization of dopant clusters.

In crystalline regions:

$$\text{Crytalline\%} = \frac{\text{FractionCryst}}{\text{DopantSize} \sum_{\text{Dopant|Cluster}} \text{FractionCryst}} \quad (479)$$

$$\begin{aligned}
 \text{MaxDopant} &= \max(\text{Dopant\_Implant} - \text{AcInit}, 0) \\
 \text{DopantCluster} &= \text{DopantCluster} + \text{Crystalline\%} \times \text{MaxDopant} \\
 \text{Dopant} &= \text{Dopant} + \text{Dopant\_Implant} - \text{MaxDopant} + \text{Crystalline\%} \times \text{MaxDopant}
 \end{aligned} \tag{480}$$

In amorphous regions:

$$\text{Amorphous\%} = \frac{\text{FractionAmor}}{\frac{\text{DopantSize}}{\sum_{\text{Dopant}|\text{DopantCluster}} \text{FractionAmor}}} \tag{481}$$

$$\begin{aligned}
 \text{MaxDopant} &= \max(\text{DopantTotal} + \text{Dopant\_Implant} - \text{AmInit}, 0) \\
 \text{DopantCluster} &= \text{Amorphous\%} \times \text{MaxDopant} \\
 \text{Dopant} &= \text{DopantTotal} + \text{Dopant\_Implant} - \text{MaxDopant} + \text{Amorphous\%} \times \text{MaxDopant}
 \end{aligned} \tag{482}$$

where:

- Dopant is the dopant name (for example, Boron).
- DopantCluster is the cluster name (for example, B4I2).
- DopantTotal is the total dopant (for example, Boron+4\*B4I2).
- Dopant\_Implant is the implanted dopant (for example, Boron\_Implant).
- DopantSize is the size of the dopant (for example, 4 for B4I2).

## Dopant Trapping at EOR Defects

To simulate dopant trapping at EOR defects [34], interstitial clusters must be switched on (311 or 2Moment), loops must be switched on, and one of the following dopant diffusion models also must be used:

- React (see [React Diffusion Model on page 183](#))
- ChargedReact (see [ChargedReact Diffusion Model on page 176](#))
- NeutralReact (see [NeutralReact Diffusion Model on page 192](#))

To switch on the model, use:

```
pdbSet <material> <dopant> EORTrap <1 | 0>
```

The following type of clustering reactions are taken into account:



## 4: Diffusion

### Dopant Activation and Clustering

where  $C_{AI}$  is the mobile dopant,  $C_{A311}$  is the concentration of mobile dopants trapped at {311} defects, and  $C_{ADL}$  is the concentration of mobile dopants trapped at dislocation loops.

For these reactions:

- The first reaction describes the capture and release of mobile dopants at {311} defects.
- The second one describes the capture and release of mobile dopants at dislocation loops.
- The last reaction explains the transformation of mobile dopants trapped at a {311} defect to mobile dopants trapped at a dislocation loop.

The capture rate for the mobile dopant and {311} defect reaction is written as:

$$R_{A311}^{capture} \equiv k_{f311}(C_{311}C_{max}^{311} - C_{A311}) \quad (486)$$

where  $k_{f311}$  is the forward reaction rate,  $C_{311}$  is the concentration of interstitials in {311} defects and  $C_{max}^{311}$  is the density of traps along the {311} defects for the mobile dopants.

To change  $k_{f311}$ , use:

```
pdbSet <material> <dopant> EORForwardReaction <trapped dopant> <n>
```

where <trapped dopant> is  $C_{A311}$  (for example, B311).

For boron, it is currently set to:

$$k_{f311} = 4\pi r_{A311} C_{AI} D_{AI} \quad (487)$$

where  $r_{A311}$  is the capture radius and  $D_{AI}$  is the diffusivity of neutral dopant–defect pair,  $C_{AI}$ .

To change the capture radius, use:

```
pdbSet <material> <dopant> EORCaptureRadius <trapped dopant> <n>
```

$C_{max}^{311}$  is proportional to the length of the {311} defect. It is defined as a term and is user definable:

```
term name= EORDopant311_Max <material> add eqn= {equation} store
```

The release rate for the mobile dopant and {311} defect reaction is written as:

$$R_{A311}^{release} \equiv C_{A311} E_{A311} \quad (488)$$

where  $E_{A311}$  is the emission rate of trapped mobile dopant from {311} defects. To change it, use:

```
pdbSet <material> <dopant> EOREmissionRate <trapped_dopant> <n>
```

The capture rate for the mobile dopant and dislocation loop reaction is written as:

$$R_{ADL}^{capture} \equiv k_{fDL}(C_{DL}C_{max}^{DL} - C_{ADL}) \quad (489)$$

where  $k_{fDL}$  is the forward reaction rate and  $C_{max}^{DL}$  is the density of traps along the edge of dislocation loops for the mobile dopants. To change  $k_{fDL}$ , use:

```
pdbSet <material> <dopant> EORForwardReaction <trapped dopant> <n>
```

where <trapped\_dopant> is  $C_{ADL}$  (for example, BDL). It is set to:

$$k_{fDL} = \pi r_{ADL} C_{AI} D_{AI} \quad (490)$$

where  $r_{ADL}$  is the capture radius. To change the capture radius, use:

```
pdbSet <material> <dopant> EORCaptureRadius <trapped_dopant> <n>
```

$C_{max}^{DL}$  is proportional to the density of dislocation loops. It is defined as a term and is user definable:

```
term name= EORDopantDL_Max <material> add eqn= {equation} store
```

The release rate for the mobile dopant and dislocation loop reaction is written as:

$$R_{ADL}^{release} \equiv C_{ADL} E_{ADL} \quad (491)$$

where  $E_{ADL}$  is the emission rate of trapped mobile dopant from a dislocation loop. To change it, use:

```
pdbSet <material> <dopant> EOREmissionRate <trapped dopant> <n>
```

The unfaulting of {311} defects in the presence of trapped mobile dopants is given as:

$$R_{A311 \rightarrow ADL}^{Unfold} \equiv K_{D311 \rightarrow DLoop} s_{311} \frac{C_{A311}}{C_{311}} \quad (492)$$

where:

- $K_{D311 \rightarrow DLoop}$  is the unfaulting rate of {311} defects to dislocation loops and comes from the Loop model (see [Defect Cluster Model: Loop on page 314](#)).
- $s_{311}$  is the size of the {311} defect.

Table 32 Solution names for EOR trap model

Symbol	Solution name
$C_{AI}$	BoronInt
$C_{A311}$	B311
$C_{ADL}$	BDL

## Initializing Dopant Trapping in EOR Model

Initially, trapped dopants at EOR are set to zero. If there is an existing cluster concentration field, the field is used. If there are amorphized regions, dopant–defect pairs and clusters are redistributed in these regions. For details, see [Initializing Dopant and Dopant–Defect Clusters on page 302](#). In addition, you can initialize any of the cluster concentration fields using the select command in the command file.

## Defect Clusters

The available cluster models are None, Equilibrium, 311, Loop, LoopEvolution, FRENDETECH, 1Moment, 2Moment, Full, and the model is selected with the command:

```
pdbSet <material> <defect> ClusterModel <model>
```

where <defect> is interstitial or vacancy, and <model> is one of the valid model names.

These clusters play an important part in transient-enhanced diffusion (TED) of impurities following ion implantation. The main effect of the models is to delay the onset of TED at low temperatures and to distribute the diffusion enhancement over a longer period of time. This eliminates the excessive diffusion at low temperatures that is predicted without any clustering.

In some cases, multiple cluster equations must be switched on. The following command can be used:

```
pdbSet <material> <defect> MultiClusterModel { <cluster model> <list> }
```

The following example switches on the 1Moment model if the interstitial cluster model Full is selected:

```
pdbSet Silicon Int MultiClusterModel { Full {1Moment}
                                         Loop {311} }
```

In the same way, it will switch on the 311 model if the interstitial cluster model Loop is selected.

The following example switches on the model given in [35]:

```
pdbSet Si Int ClusterModel Full
pdbSet Si Int MultiClusterModel Full {2Moment Loop}
```

In this model, seven equations are solved to describe the kinetics of self-interstitial clusters:

- Three data fields ( $I_2$ ,  $I_3$ ,  $I_4$ ) describe small interstitial clusters (SMICs).
- Two data fields ( $D_{311}$ , density of  $\{311\}$  defects, and  $C_{311}$ , density of interstitials bound in  $\{311\}$  defects) describe the presence of  $\{311\}$  defects.
- Two data fields ( $D_{Loop}$ , density of dislocation loops, and  $C_{Loop}$ , density of interstitials bound in dislocation loops) describe dislocation loops.

## Defect Cluster Model: None

If `ClusterModel` is set to `None`, no point-defect clustering effects will be taken into account.

## Defect Cluster Model: Equilibrium

If you set the model to `Equilibrium`, the following nonlinear algebraic equation along with the related diffusion equations are solved:

$$(C_X^0)^4 - k_b C_{XC} = 0 \quad (493)$$

where  $k_b$  is the equilibrium constant,  $X$  is either interstitial or vacancy, 4 is the size of the cluster, and  $C_{XC}$  is the concentration of point-defect cluster.  $k_b$  can be specified with:

```
pdbSet <material> <defect> KCluster {<n>}
```

**NOTE** The equilibrium cluster model is defined only for interstitials in silicon.

## Defect Cluster Model: 311

If you set the defect cluster model to `311`, the  $\{311\}$  point-defect model developed by Law and Jones [36] is activated. It solves for the concentration of interstitials in the defects  $C_{311}$  and the concentration of defects  $D_{311}$ , as well as for the concentration of interstitials in small interstitial clusters (SMICs).

SMICs come in two types. The small type *SmicS* is assumed to have a cluster size of 2. The larger type *Smic* is assumed to have a cluster size of  $N_{size} = 4$ , by default.

## 4: Diffusion

### Defect Clusters

This value is, however, user accessible:

```
pdbSet <material> C311 NSize {<n>}
```

Nucleation of defects occurs during the implantation process. Initial distribution of defects comes from the implantation code (see [Ion Implantation to Diffusion on page 339](#)), in particular, all interstitials created during the implantation process are assumed to be in immobile *SmicS*. Vacancies and interstitials recombine or may form di-interstitials and di-vacancies. Some interstitials will also form small interstitial clusters (*SmicS*, *Smic*) or {311} defects. The SMICs dissolve to the surface through the release of interstitials. The capture and release of interstitials on the {311} defects occur only at the end of the defects and, therefore, are proportional to the number of defects  $D_{311}$ .

The reactions involved in the {311} model are given by:



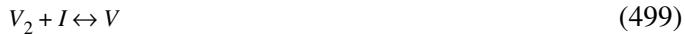
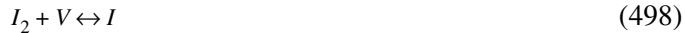
$$R_{I_2form} = k_f(C_I^2 - B_{I_2}C_I) \quad (496)$$

$$R_{V_2form} = k_f(C_V^2 - B_{V_2}C_V) \quad (497)$$

where  $I_2$  and  $V_2$  are di-interstitials and di-vacancies, and  $B_{X_2}$  is the binding coefficient between the di-defect, for example,  $I_2$ , and the base defect,  $I$  (where  $X$  refers to either I or V), and  $k_f$  is the forward reaction rate for the recombination of di-defects.

To change these variables, use the commands:

```
pdbSet <material> <di-defect> Kforward {<n>}
pdbSet <material> <di-defect> Bind {<n>}
```



$$R_{I_2rec} = k_f \left( C_{I_2} C_V - C_{I_2}^* C_V^* \frac{C_I}{C_I^*} \right) \quad (501)$$

$$R_{V_2rec} = k_f \left( C_{V_2} C_I - C_{V_2}^* C_I^* \frac{C_V}{C_V^*} \right) \quad (502)$$

$$R_{I_2V_2rec} = k_f(C_{I_2}C_{V_2} - C_{I_2}^*C_{V_2}^*) \quad (503)$$

where  $C_X^*$  is the equilibrium concentration of the respective defect or di-defect, and  $k_f$  is the forward reaction rate for the respective recombination process.

To change these variables, use the commands:

```
pdbSet <material> <di-defect> KRecomb {<n>}
pdbSet <material> <di-defect> KBiMole {<n>}
pdbSet <material> <di-defect> Cstar {<n>}
```

Aggregation or emission of interstitials from  $SmicS$  and  $Smic$  are given by:



$$R_{ISmicSagg} = k_{fl}C_{SmicS}(C_I - B_{ISmicS}) \quad (505)$$

This process increases the concentration of interstitials in  $SmicS$  by  $1/\text{cm}^3$ .



$$R_{ISmicagg} = k_{fl}C_{Smic}(C_I - B_{ISmic}) \quad (507)$$

This process increases the concentration of interstitials in  $Smic$  by  $1/\text{cm}^3$ .  $k_{fl}$  is the forward reaction rate for SMIC–interstitial reactions, and  $B_{ISmicS}$  and  $B_{ISmic}$  are the binding coefficients between interstitials and SMICs.

To change these variables, use the commands:

```
pdbSet <material> SmicS KfI {<n>}
pdbSet <material> SmicS Bind {<n>}
pdbSet <material> Smic KfI {<n>}
pdbSet <material> Smic Bind {<n>}
```

The recombination of  $SmicS$  or  $Smic$  with a vacancy or bi-vacancies is given by:



$$R_{VSmicSrec} = k_{fV}C_VC_{SmicS} \quad (509)$$

This process decreases the concentration of interstitials in  $SmicS$  by  $1/\text{cm}^3$ .



$$R_{VSmicrec} = k_{fV}C_VC_{Smic} \quad (511)$$

## 4: Diffusion

### Defect Clusters

This process decreases the concentration of interstitials in  $Smic$  by  $1/cm^3$ .



$$R_{V_2 SmicS rec} = k_{fV_2} C_{V_2} C_{SmicS} \quad (513)$$

This process decreases the concentration of interstitials in  $SmicS$  by  $2/cm^3$ .



$$R_{V_2 Smic rec} = k_{fV_2} C_{V_2} C_{Smic} \quad (515)$$

This process decreases the concentration of interstitials in  $Smic$  by  $2/cm^3$ .  $k_{fV}$  and  $k_{fV_2}$  are the diffusion-limited SMIC-(di-)vacancy capture rates and are defined as:

$$k_{fV} = 4\pi a D_{V^0} \quad (516)$$

$$k_{fV} = 4\pi a D_{V_2^0} \quad (517)$$

where:

- $D_{V^0}$  and  $D_{V_2^0}$  are the diffusivities of neutral vacancies and di-vacancies.
- $a$  is the lattice spacing of silicon.

To change these variables, use the commands:

```

pdbSet <material> Vacancy D 0      {<n>}
pdbSet <material> V2      D0      {<n>}
pdbSet <material> LatticeSpacing {<n>}
```

A  $Smic$  is assumed to contain  $N_{size}$  interstitials, with a default value of 4. A  $SmicS$  contain two interstitials less than a  $Smic$ . A  $SmicS$  can be converted to a  $Smic$  by combining with a di-interstitial. Formation of a  $Smic$  from a  $SmicS$  and bi-interstitials is given by:



$$R_{Smicform} = k_{fl_2} C_{SmicS} C_{I_2} \quad (519)$$

This process increases the concentration of interstitials in  $Smic$  by  $N_{size}/cm^3$  and decreases the concentration of interstitials in  $SmicS$  by  $(N_{size} - 2)/cm^3$ .  $k_{fl_2}$  is the forward reaction rate for SMIC-di-interstitial reactions. To change these variables, use:

```

pdbSet <material> SmicS KfI2  {<n>}
pdbSet <material> C311  NSize {<n>}
```

When a *Smic* combines with an additional di-interstitial, they form a {311} defect. Formation of a new {311} defect from a *Smic* and bi-interstitials is given by:



$$R_{311nIform} = k_{nI_2} C_{Smic} C_{I_2} \quad (521)$$

This process increases the concentration of {311} defects by  $1/\text{cm}^3$  and the concentration of interstitials in {311} defects by  $(N_{size} + 2)/\text{cm}^3$ , and deceases the number of interstitials in a *Smic* by  $N_{size}/\text{cm}^3$ .  $k_{nI_2}$  is the reaction rate.

To change these variables, use:

```
pdbSet <material> C311 KnI2 {<n>}
```

The emission of interstitials from {311} defects is given by:



$$R_{C_{311}Iem} = C_{311} D_{Rate} \quad (523)$$

This process decreases the concentration of interstitials in {311} defects by  $1/\text{cm}^3$ , but does not change the number of {311} defects. The {311} defect simply became shorter.  $C_{311}$  is the concentration of interstitials in the {311} defects and  $D_{Rate}$  is the decay rate.

To change these variables, use the commands:

```
pdbSet <material> C311 Decay {<n>}
```

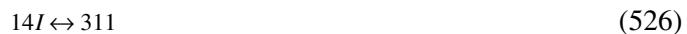
The dissolution of a defect is given by:



$$R_{D_{311}decay} = D_{311} D_{Rate} \quad (525)$$

This process changes the number of {311} defects, but does not affect the number of interstitials in the {311} defects. The interstitials released in this process immediately aggregate on other {311} defects.  $D_{311}$  is the concentration of {311} defects and  $D_{Rate}$  is the defect decay rate.

A set of 14 interstitials can nucleate at the end of a {311} defect. The formation or dissolution of a {311} defect from interstitials is given by:



## 4: Diffusion

### Defect Clusters

$$R_{C_{311}Iform} = k_{fl}D_{311}14R_I(C_I - B_{D_{311}I}) \quad (527)$$

This process increases the concentration of interstitials in {311} defects by  $14/\text{cm}^3$ ; the number of defects remains unchanged.  $k_{fl}$  is the forward reaction rate,  $R_I$  is the capture (reaction) range, and  $B_{D_{311}I}$  is the binding coefficient between the {311} defect and the interstitial. To change these variables, use:

```

pdbSet <material> C311 KfI      {<n>}
pdbSet <material> C311 BindI    {<n>}
pdbSet <material> C311 RangeI   {<n>}

```

A set of 14 di-interstitials can nucleate at the end of a {311} defect. The formation of two {311} defects from seven bi-interstitials is given by:



$$R_{C_{311}I_2form} = D_{311}k_{fl_2}14R_{I_2}(C_{I_2} - B_{D_{311}I_2}) \quad (529)$$

This process increases the concentration of interstitials in {311} defects by  $28/\text{cm}^3$ ; the number of defects remains unchanged.  $k_{fl_2}$  is the forward reaction rate,  $R_{I_2}$  is the capture (reaction) range, and  $B_{D_{311}I_2}$  is the binding coefficient between the {311} defect and the interstitial. To change these variables, use:

```

pdbSet <material> C311 BindI2   {<n>}
pdbSet <material> C311 KfI2     {<n>}
pdbSet <material> C311 RangeI2  {<n>}

```

A {311} defect can dissolve into interstitials or di-interstitials. The probability of this process is proportional to the inverse length of the defect, which can be expressed as the ratio of the concentration of defects and the concentration of interstitials in defects ( $D_{311}/C_{311}$ ). Then, the dissolution of {311} defects is given by:

$$R_{D_{311}Iem} = D_{311}14C_{Rate}\frac{D_{311}}{C_{311}}k_{fl}R_I B_{D_{311}I} \quad (530)$$

$$R_{D_{311}I_2em} = D_{311}14C_{Rate}\frac{D_{311}}{C_{311}}k_{fl_2}R_{I_2}B_{D_{311}I_2} \quad (531)$$

This process does not change the number of free interstitials or the number of interstitials in {311} defects. It is assumed that all interstitials were released from the defect aggregate in other {311} defects.  $C_{Rate}$  is the spontaneous combustion rate and gives the percentage of interstitials dissolved from {311} defects by dissolution of all defects. To change these variables, use:

```

pdbSet <material> C311 CombRate {<n>}

```

The following set of differential equations is solved with the {311} model. The point-defect equations are:

$$\begin{aligned}\frac{\partial C_I}{\partial t} = & -\nabla \bullet J_I - R_{IV} - 2R_{I_2form} + R_{I_2rec} - R_{V_2rec} - R_{C_{311}Ifom} \\ & + R_{C_{311}Iem} - R_{ISmicSagg} - R_{ISmicagg}\end{aligned}\quad (532)$$

$$\frac{\partial C_V}{\partial t} = -\nabla \bullet J_V - R_{IV} - 2R_{V_2form} + R_{V_2rec} - R_{I_2rec} - R_{VSmicSrec} - R_{VSmicrec}\quad (533)$$

The di-defect equations are:

$$\frac{\partial C_{I_2}}{\partial t} = \nabla \bullet (D_{I_2} \nabla C_{I_2}) + R_{I_2form} - R_{I_2rec} - R_{I_2V_2rec} - R_{Smicform} - R_{311nIfom} - R_{C_{311}I_2form}\quad (534)$$

$$\frac{\partial C_{V_2}}{\partial t} = \nabla \bullet (D_{V_2} \nabla C_{V_2}) + R_{V_2form} - R_{V_2rec} - R_{I_2V_2rec} - R_{V_2SmicSrec} - R_{V_2Smicrec}\quad (535)$$

where  $D_{X_2}$  is the diffusivities of di-defects (where X refers to either I or V).

To change these variables, use:

```
pdbSet <material> <di-defect> D0 {<n>}
```

The equation for  $SmicS$  is given by:

$$\frac{\partial C_{SmicS}}{\partial t} = -R_{VSmicSrec} - 2R_{V_2SmicSrec} + R_{ISmicSagg} - R_{Smicform}\quad (536)$$

The equation for  $Smic$  is given by:

$$\frac{\partial C_{Smic}}{\partial t} = -R_{VSmicrec} - 2R_{V_2Smicrec} + R_{ISmicagg} + R_{Smicform}N_{Size} + R_{311nIfom}N_{Size}\quad (537)$$

The equation for the density of {311} defects is given by:

$$\frac{\partial C_{D_{311}}}{\partial t} = -R_{D_{311}decay} - R_{D_{311}Iem} - 2R_{D_{311}I_2em} + R_{311nIfom}\quad (538)$$

The equation for the concentration of interstitials in {311} defects is given by:

$$\frac{\partial C_{C_{311}}}{\partial t} = -R_{C_{311}Iem} + R_{C_{311}Ifom} + 2R_{C_{311}I_2fom} + (N_{size} + 2)R_{311nIfom}\quad (539)$$

The initialization of {311} defect fields is given in [Ion Implantation to Diffusion on page 339](#).

Table 33 Solution names for 311 model

Symbol	Solution name
$C_{311}$	C311
$D_{311}$	D311
$C_{Smic}$	Smic
$C_{SmicS}$	SmicS
$C_{I_2}$	I2
$C_{V_2}$	V2

**NOTE** Even though the 311 model and the model parameters are given in general format, they are defined only for silicon. If these models must be used in other materials, their parameters must be copied.

## Initializing 311 Model

The defect-cluster concentrations I2, V2, C311, SmicS, Smic, and D311 are initialized in the diffPreProcess procedure. The model assumes that all the free implantation interstitials (Int\_Implant) are transferred to SmicS. Initially, other transient defect-cluster concentrations are set to zero. If there is an existing cluster concentration field, the field is used. By default, clusters are assumed to break apart in the amorphous regions. You can specify the percentage of clusters retained in the amorphous region per cluster solution variable using the parameter AmPercent:

```
pdbSet <mater> <cluster> AmPercent {<n>}
```

For example:

$$SmicS = \begin{cases} SmicS * AmPercent & \text{Amorphous regions} \\ SmicS + Int\_Implant & \text{Crystalline regions} \end{cases} \quad (540)$$

$$C_{311} = \begin{cases} C_{311} * AmPercent & \text{Amorphous regions} \\ C_{311} & \text{Crystalline regions} \end{cases} \quad (541)$$

The value of the AmPercent parameter must be between 0 and 1.

## Defect Cluster Model: Loop

If you set the defect cluster model to Loop, the modified version of the dislocation loop nucleation model [37] is used to solve for the concentration of interstitials in the defects  $C_{Loop}$

and the concentration of defects  $D_{Loop}$ . The model assumes that the dislocation loops come from unfaulted {311} defects. The unfaulting rate can be defect size-dependent or not.

The following switch can be used to change the unfaulting rate:

```
pdbSet <material> CLoop Unfault.Model <model>
```

where <model> is either Direct or SizeDependent.

## Direct Model

If the Unfault.Model is set to Direct, the following reaction equations as well as the {311} defect equations (see [Defect Cluster Model: 311 on page 307](#)) are solved:

$$\frac{\partial C_{Loop}}{\partial t} = K_{311}C_{311} + 2\pi^2 R_{Loop} D_{Loop} D_{I^0} K_{CLoop} (C_I - C_{ILoop}^*) \quad (542)$$

$$C_{ILoop}^* \equiv C_I^* e^{\left(\frac{\gamma\Omega}{bkT}\right) \left(\frac{\mu b\Omega}{4\pi R_{Loop} kT(1-\nu)} \ln\left(\frac{8R_{Loop}}{b}\right)\right)} \quad (543)$$

$$\frac{\partial D_{Loop}}{\partial t} = K_{311}D_{311} - K_{DLoop} \frac{2D_{Loop}}{R_{Loop}^2} \quad (544)$$

where:

- $K_{311}$  is the unfaulting rate of {311} defects to dislocation loops.
- $R_{Loop}$  is the average radius of loops.
- $D_{I^0}$  is the diffusivity of neutral interstitials.
- $\mu$  is the shear modulus (dyn/cm<sup>2</sup>).
- $\gamma$  is the stacking fault energy (dyn/cm).
- $\Omega$  is the atomic value of silicon ( $2 \times 10^{-23}$ ).
- $\nu$  is the Poisson ratio.
- $b$  is the magnitude of the Burgers vector.
- $K_{CLoop}$  and  $K_{DLoop}$  are fitting parameters for the model.

These parameters can be set using the following commands:

```
pdbSet <material> CLoop      K311          {<n>}
pdbSet <material> Mechanics  ShearModulus   {<n>}
pdbSet <material> CLoop      Stacking.Fault.Energy {<n>}
pdbSet <material> CLoop      Burgers.Vector    {<n>}
pdbSet <material> CLoop      KCLoop         {<n>}
pdbSet <material> DLoop      KDLoop         {<n>}
```

## Size-Dependent Model

If the `Unfault.Model` is set to `SizeDependent`, the following reaction equations and the {311} defect equations (see [Defect Cluster Model: 311 on page 307](#)) are solved:

$$\frac{\partial C_{Loop}}{\partial t} = K_{311} C_{311}^2 C_T + 2\pi^2 R_{Loop} D_{Loop} D_{I^0} K_{CLoop} (C_I - C_{ILoop}^*) \quad (545)$$

$$\frac{\partial D_{Loop}}{\partial t} = K_{311} D_{311} C_{311} C_T K_{D311} - \frac{2\pi^2 R_{Loop} D_{Loop}^2 D_{I^0} K_{CLoop} C_{ILoop}^*}{C_{Loop}} \quad (546)$$

where  $K_{D311}$  is the scaling factor for the unfaulting rate and can be defined using the command:

```
pdbSet <material> CLoop KD311 {<n>}
```

$C_T$  is the user-defined term to further modify the unfaulting rate and can be defined using the command:

```
term name= CLoopTransfer <material> eqn= {user-defined equation} store
```

The model is used to simulate all three phases of dislocation nucleation and evolution: nucleation, Ostwald ripening, and dissolution.

To modify the equilibrium concentration of interstitials at the loop boundaries ( $C_{ILoop}^*$ ) by complex prefactors, you can define the following terms in the command file:

```
term name= CLoopDissIntFactor silicon add eqn= {equation} store
```

$C_{ILoop}^*$  increases dramatically as the loop radius becomes smaller. To avoid convergence problems,  $C_{ILoop}^*$  is limited by a minimum loop radius ( $R_{LoopMin}$ ) and  $C_{Loop}^{dFactor}$  as follows:

$$C_{ILoop}^* = \frac{C_{ILoop}^*(R_{LoopMin}) C_{ILoop}^*(R_{Loop})}{C_{ILoop}^*(R_{LoopMin}) + C_{ILoop}^*(R_{Loop})} \left( 1 - \frac{C_{Loop}^{dFactor}}{C_{Loop} + C_{Loop}^{dFactor}} \right) \quad (547)$$

The minimum radius and the damping factor are set with the commands:

```
pdbSet <material> CLoop RLoopMin {<n>}
pdbSet <material> CLoop DampFactor {<n>}
```

If the Loop model is used with the 2Moment model, to avoid convergence problems, the interstitial evaporation terms in [Eq. 585](#), [Eq. 586](#), [Eq. 587](#), and [Eq. 588](#) are scaled by:

$$R_{limit} = \left( 1 - \frac{C_{311}^{dFactor}}{C_{311}^{dFactor} + C_{311}} \right) \quad (548)$$

The damping factor for the {311} defects can be set:

```
pdbSet <material> C311 DampFactor {<n>}
```

Table 34 Solution names for loop model

Symbol	Solution name
$C_{Loop}$	CLoop
$D_{Loop}$	DLoop

## Initializing Loop Model

Since the loop model relies on the {311} defect model, first, the {311} defect model is initialized (see [Initializing 311 Model on page 314](#)). Then, the loop model fields CLoop and DLoop are initialized. If there is no preexisting data field, the fields are set to  $1 \times 10^{10}$  and  $5 \times 10^7$ , respectively. If there is an existing data field, the existing fields are used. By default, the loops are assumed to break apart in the amorphous regions.

You can specify the percentage of loops retained in the amorphous region per solution variable using the parameter AmPercent:

```
pdbSet <mater> DLoop AmPercent {<n>}  
pdbSet <mater> CLoop AmPercent {<n>}
```

For example:

$$D_{Loop} = \begin{cases} D_{Loop} * \text{AmPercent} & \text{Amorphous regions} \\ D_{Loop} & \text{Crystalline regions} \end{cases} \quad (549)$$

$$C_{Loop} = \begin{cases} C_{Loop} * \text{AmPercent} & \text{Amorphous regions} \\ C_{Loop} & \text{Crystalline regions} \end{cases} \quad (550)$$

The value of the AmPercent parameter must be between 0 and 1.

## Defect Cluster Model: LoopEvolution

If you set the defect cluster model to LoopEvolution, the TSUPREM-4-style loop evolution model [38] is used. The rate of absorption of interstitials by dislocation loops is given by:

$$R_I \equiv 2\pi^2 R_{Loop} K_{CLoop} D_{Loop} D_I (C_I - C_{ILoop}^*) \quad (551)$$

$$C_{ILoop}^* \equiv C_I^* e^{\left(\frac{\gamma\Omega}{b k T}\right)} e^{\left(\frac{\mu b \Omega}{4\pi R_{Loop} k T (1-\nu)} \ln\left(\frac{8R_{Loop}}{b}\right)\right)} \quad (552)$$

where:

- $R_{Loop}$  is the average loop radius.
- $D_{Loop}$  is the loop density.
- $D_I$  is the diffusivity of interstitials.
- $K_{CLoop}$  is the fitting parameter.
- $\mu$  is the shear modulus (dyn/cm<sup>2</sup>).
- $\gamma$  is the stacking fault energy (dyn/cm).
- $\Omega$  is the atomic value of silicon ( $2 \times 10^{-23}$ ).
- $\nu$  is the Poisson ratio.
- $b$  is the magnitude of the Burgers vector.

These parameters can be set using the following commands:

```
pdbSet <material> CLoop ShearModulus      {<n>}
pdbSet <material> CLoop Stacking.Fault.Energy {<n>}
pdbSet <material> CLoop Burgers.Vector      {<n>}
pdbSet <material> CLoop KCLoop             {<n>}
```

The evolution of the loop radius is given by:

$$\frac{\partial R_{Loop}}{\partial t} = \frac{\pi}{N_0} K_{CLoop} D_I (C_I - C_{ILoop}^*) \quad (553)$$

where  $N_0$  is the {111} planar density of silicon ( $1.57 \times 10^{15}$  cm<sup>-2</sup>).

The equilibrium concentration of interstitials at the loop boundaries ( $C_{ILoop}^*$ ) increases dramatically as the loop radius becomes smaller. To avoid convergence problems,  $R_I$  is limited by a minimum loop radius ( $R_{LoopMin}$ ) as follows:

$$Damp_0 \equiv \frac{R_{Loop}}{R_{LoopMin}}; \quad Damp \equiv \frac{Damp_0(4.605)}{Damp_0 + 4.605} \quad (554)$$

$$R_I \equiv R_I(R_{Loop})(1 - e^{-(Damp)})$$

To set the minimum radius, use:

```
pdbSet <material> CLoop RLoopMin {<n>}
```

To set the density of loops to a fixed value, use:

```
pdbSet <mater> DLoop ConstantDensity {<n>}
```

Table 35 Solution names for LoopEvolution model

Symbol	Solution name
$R_{Loop}$	RLoop

## Initializing LoopEvolution Model

To specify the initial loop radius, use:

```
pdbSet <mater> RLoop InitialRadius {<n>}
```

To set the density of loops to a fixed value, use:

```
pdbSet <mater> DLoop ConstantDensity {<n>}
```

or it will be calculated using the following:

$$D_{Loop} = \frac{Fraction(C_I - Threshold)}{\pi N_0 R_{Loop}^2} \quad (555)$$

where Fraction and Threshold can be set with:

```
pdbSet <material> CLoop Fraction {<n>}  
pdbSet <material> CLoop Threshold {<n>}
```

**NOTE** If ConstantDensity is zero, Eq. 555 will be used.

Loops are produced in that portion of the structure where the interstitial concentration (due to implantation damage, before recombination) is in the range:

$D_{max} > Damage > D_{min}$  (556)

$D_{max}$  and  $D_{min}$  can be set:

```
pdbSet <material> CLoop Dmin {<n>}  
pdbSet <material> CLoop Dmax {<n>}
```

The concentration of interstitials corresponding to the edge of the amorphous region is from the work of Fair and Pappas [3]. The concentration of interstitials is not reduced by the formation of end-of-range loops if DLoop is set to a constant value. Pre-existing dislocation loops in the region are presumed to be destroyed by the implantation.

**NOTE** In this model, CLoop and DLoop are terms. Therefore, they must be either converted to data fields with the select command or added to the plx/TDR list to save in a file.

## Defect Cluster Model: FRENDTECH

If you set the model to FRENDTECH, this activates the extended defect model developed by FRENDTECH partners [39][40][41]. The model assumes the following reactions:



where  $I_n$  and  $I_{n+1}$  are the interstitial defects consisting of  $n$  and  $n+1$  silicon atoms. The reactions can be written as:

$$R_1 \equiv k_{f_{n-1}} C_{I_{n-1}} - k_{r_n} C_{I_n} \quad (559)$$

$$R_2 \equiv -(k_{f_n} C_{I_n} - k_{r_{n+1}} C_{I_{n+1}}) \quad (560)$$

and the model is given by:

$$\frac{\partial C_{I_n}}{\partial t} = R_1 + R_2 \quad (561)$$

where  $C_{I_n}$  is the density of defects containing  $n$  atoms.

The emission rate  $k_{r_n}$  is given by:

$$k_{r_n} = D_{I^0} C_I^* \frac{A_{n-1}}{R_{\text{eff}}} e^{\left(\frac{+E_{fn}}{kT}\right)} \quad (562)$$

where:

- $D_{I^0}$  is the diffusion coefficient of neutral interstitials.
- $C_I^*$  is the equilibrium concentration of interstitials.
- $\frac{A_{n-1}}{R_{\text{eff}}}$  is the capture efficiency of the defect.
- $E_{fn}$  is its formation energy.

The capture rate  $k_{f_n}$  is:

$$k_{f_n} = D_{I^0} C_I \frac{A_n}{R_{\text{eff}}} \quad (563)$$

where  $C_I$  is the concentration of interstitials.

$A_n/R_{\text{eff}}$  and  $E_{fn}$  can be defined using the command:

```
pdbSet <material> Interstitial Bind.Cluster <cluster> {<n>}
```

where `<cluster>` is a valid cluster name (for example, `I2`, `I3`, `I21`) and `<n>` must be an Arrhenius expression with a prefactor of  $A_n/R_{\text{eff}}$  and an activation energy of  $E_{fn}$ .

The following example sets  $A_n/R_{\text{eff}}$  to  $3.82578 \times 10^{-7}$  eV and  $E_{fn}$  to  $-1.29$  eV for  $n = 6$ :

```
pdbSet Silicon Interstitial Bind.Cluster I6 {[Arrhenius 3.82578e-07 -1.29]}
```

Since cluster sizes can change easily from a few atoms to a few thousand atoms, it is not feasible to solve all cluster equations. Therefore, the number of equations to be solved is reduced by using the method proposed by FRENDETECH partners [42]. The method allows for the logarithmic discretization of clusters:

$$\begin{aligned} \frac{d}{dt}\rho(u) = & -\left(1 + \frac{e^{-u}}{2}\right)\frac{e^{-u}}{2\alpha}(k_{F_{u+\alpha}}\rho_{u+\alpha} - k_{F_{u-\alpha}}\rho_{u-\alpha}) \\ & +\left(1 - \frac{e^{-u}}{2}\right)\frac{e^{-u}}{2\alpha}(k_{R_{u+\alpha}}\rho_{u+\alpha} - k_{R_{u-\alpha}}\rho_{u-\alpha}) \\ & +\frac{e^{-2u}}{2\alpha^2}(k_{F_{u+\alpha}}\rho_{u+\alpha} - 2k_{F_u}\rho_u + k_{F_{u-\alpha}}\rho_{u-\alpha}) \\ & +\frac{e^{-2u}}{2\alpha^2}(k_{R_{u+\alpha}}\rho_{u+\alpha} - 2k_{R_u}\rho_u + k_{R_{u-\alpha}}\rho_{u-\alpha}) \end{aligned} \quad (564)$$

where  $\rho(u)$  is the density function, and  $\alpha$  is the step of the logarithmic discretization.  $k_{F_u}$  and  $k_{R_u}$  are related to the capture and emission rate  $k_{f_n}$  and  $k_{r_n}$  by the relations:

$$k_{F_u} = k_{f_{n=e^u}} \quad (565)$$

$$k_{R_u} = k_{r_{n=e^u}} \quad (566)$$

The discretization is regular on a regularities scale. For example, the step in the reduced region is calculated by:

$$\alpha = \frac{\log(n_{\text{max}}(-1)) - \log(n_{\text{lastlin}} + 1)}{n_{\text{logsteps}}} \quad (567)$$

where  $n_{\text{max}}$  is the biggest cluster size,  $n_{\text{lastlin}}$  is the number of small interstitial clusters in the linear region, and  $n_{\text{logsteps}}$  is the number of steps in the reduced region. You can specify  $n_{\text{max}}$ ,  $n_{\text{lastlin}}$ , and  $n_{\text{logsteps}}$  using the following commands:

```
pdbSet <material> Int Biggest.Cluster.Size {<n>}
pdbSet <material> Int Number.Of.Small.Clusters {<n>}
pdbSet <material> Int Log.Steps {<n>}
```

## 4: Diffusion

### Defect Clusters

The following example allows Sentaurus Process to solve the cluster equations for I2, I3, I4, I5, I6, I7, I8, I9, I10, I11, I12, I46, I177, I679, I2605, and I10000:

```
pdbSet Silicon Int Biggest.Cluster.Size      10000
pdbSet Silicon Int Number.Of.Small.Clusters 11
pdbSet Silicon Int Log.Steps                5
```

The capture and emission rate  $k_{f_n}$  and  $k_{r_n}$  are stored in the parameter database for cluster sizes less than 10. If you do not specify the rates for bigger clusters, they will be calculated using the following formulas:

$$\frac{A_n}{R_{eff}} \Big|_{\{311\}} = \frac{4\pi aL + 4\pi aW + 8\pi a^2}{\log\left(1 + \sqrt{1 + \left(\frac{2a}{W}\right)^2}\right) - \log\left(\frac{2a}{W}\right) + \log\left(1 + \sqrt{1 + \left(\frac{2(L+a)}{W}\right)^2}\right) - \log\left(\frac{2(L+a)}{W}\right)} \quad (568)$$

$$\frac{1}{a} \sqrt{1 + \left(\frac{2a}{W}\right)^2} + \frac{1}{L+a} \sqrt{1 + \left(\frac{2(L+a)}{W}\right)^2}$$

$$E_{strain}^n = \frac{\mu b^2 L}{2\pi(1-\nu)} \log\left(\frac{2W}{b}\right) + \frac{\mu b^2 W}{2\pi} \left( (\cos\theta)^2 + \left(\frac{(\sin\theta)^2}{1-\nu}\right) \right) \log\left(\frac{2L}{b}\right) \quad (569)$$

$$E_{fn} = E_{strain}^{n+1} + \gamma \cdot (n+1) - E_{strain}^n + \gamma \cdot n \quad (570)$$

where:

- $L$  and  $W$  are the length and width of the  $\{311\}$  defect ( $L = n \cdot 5 \times 10^{-9}$  cm and  $W = 4 \times 10^{-7}$  cm).
- $a$  is the lattice spacing of silicon.
- $\mu$  denotes the shear modulus of silicon ( $\mu = 7.55 \times 10^{11}$  dyn/cm).
- $\nu$  is the Poisson ratio ( $\nu = 0.3$ ).
- $b$  is the length of the Burgers vector ( $b = 1.1 \times 10^{-8}$  cm).
- $\theta$  is the angle between the Burgers vector and the normal vector perpendicular to the plane of the defect ( $\theta = 77.8^\circ$ ).
- $\gamma$  is the stacking fault energy per atom ( $\gamma = 0.38$  eV).

The Burgers vector and the stacking fault energy can be set using the commands:

```
pdbSet <material> C311 Burgers.Vector      {<n>}
pdbSet <material> Int Stacking.Fault.Energy {<n>}
```

Table 36 Solution names for FRENDETECH model

Symbol	Solution name
$C_{I_2}$	I2
$C_{I_3}$	I3
$C_{I_{10}}$	I10

**NOTE** Since FRENDETECH models solve for a range of cluster sizes, simulations may be slower.

## Initializing FRENDETECH Model

By default, the interstitial clusters are assumed to break apart in amorphous regions. You can specify the percentage of clusters retained in the amorphous region per solution variable using the parameter AmPercent:

```
pdbSetDouble <mater> I200 AmPercent {<n>}
pdbSetDouble <mater> I100 AmPercent {<n>}
```

For example:

$$I_{200} = \begin{cases} I_{200} * \text{AmPercent} & \text{Amorphous regions} \\ I_{299} & \text{Crystalline regions} \end{cases} \quad (571)$$

Since not all clusters have been incorporated into the parameter database, the `pdbSetDouble` command must be used; the shorthand `pdbSet` command cannot be used to specify these parameters. The value specified for the `AmPercent` parameter must be between 0 and 1.

## Defect Cluster Model: 1Moment

### Interstitial

If you set the model to `1Moment`, the model for the formation and dissolution of interstitial clusters (`{311}` or `{113}` defects) is included. The `1Moment` model uses a single equation to calculate the total number of interstitials bound in clusters. The following nonlinear algebraic equation along with the related diffusion equations are solved:

$$\frac{\partial C_{ICluster}}{\partial t} = R_{CI} - R_{CV} \quad (572)$$

where  $C_{ICluster}$  is the concentration of clustered interstitials, and  $R_{CI}$  and  $R_{CV}$  describe cluster interaction with interstitials and vacancies, respectively.

## 4: Diffusion

### Defect Clusters

The interstitial interaction includes two terms describing the clustering of interstitials and one describing the de-clustering:

$$R_{CI} = I_{kfi} \frac{(C_I)^{I_{fi}}}{(C_I^*)^{I_{sfi}}} + I_{kfc} \frac{(C_I)^{I_{fc}}}{(C_I^*)^{I_{sfc}}} (C_{ICluster} + I_{kfc} C_I) - I_{kr} (C_{ICluster})^{I_{cr}} \quad (573)$$

where  $C_I$  is the concentration of unclustered interstitials, and  $C_I^*$  is the equilibrium concentration of interstitials. The first term models nucleation of the interstitial clusters at high interstitial supersaturation. The second term models growth of the interstitial clusters by consuming free interstitials. The third term models dissolution of the interstitial clusters by emitting interstitials. If the 1Moment model is used with the Full cluster model, Eq. 573 is modified as follows:

$$R_{CI} = (max + 1) R_{sIcl(max+1)} + I_{kfc} \frac{(C_I)^{I_{fc}}}{(C_I^*)^{I_{sfc}}} (C_{ICluster} + I_{kfc} C_I) - I_{kr} (C_{ICluster})^{I_{cr}} \quad (574)$$

where  $R_{sIcl(max+1)}$  is given in [Defect Cluster Model: Full on page 332](#). The smallest large cluster forms when the small cluster captures one free interstitial by the reaction rate  $R_{sIcl(max+1)}$ . The vacancy interaction includes one recombination and one generation term:

$$R_{CV} = V_{krv} \frac{(C_V)^{V_{rv}}}{(C_V^*)^{V_{srv}}} (C_{ICluster})^{V_{crv}} - V_{kf} (C_V^*)^{V_{sfv}} (C_{ICluster})^{V_{cfv}} \quad (575)$$

where  $C_V$  is the concentration of free vacancies and  $C_V^*$  is the equilibrium concentration of vacancies. The first term models dissolution of the interstitial clusters by consuming vacancies. The second term models the emission of vacancies by the interstitial clusters.

To modify the dissolution rates  $I_{kr}$  and  $V_{kf}$  by complex prefactors, you can define the following terms in the input file:

```
term name= IClusterDissIntFactor silicon add eqn= {equation} store
term name= IClusterDissVacFactor silicon add eqn= {equation} store
```

For extrinsic silicon, the prefactors can be made a function of  $\left(\frac{n}{n_i}\right)$  to provide consistent TED results.

If the 1Moment model is used with the Full cluster model, Eq. 575 is modified as follows:

$$R_{CV} = (max + 1) R_{sIcv(max+1)} + V_{krv} \frac{(C_V)^{V_{rv}}}{(C_V^*)^{V_{srv}}} (C_{ICluster})^{V_{crv}} - V_{kf} (C_V^*)^{V_{sfv}} (C_{ICluster})^{V_{cfv}} \quad (576)$$

where  $R_{sIcV(max+1)}$  is given in [Defect Cluster Model: Full on page 332](#). It is the reaction rate of small interstitial clusters with vacancies. The reaction constants of the model can be modified using the following commands:

```

pdbSet <material> ICluster Ikfi  {<n>}
pdbSet <material> ICluster Ikfc  {<n>}
pdbSet <material> ICluster Ikr   {<n>}
pdbSet <material> ICluster Ifi   {<n>}
pdbSet <material> ICluster Isfi  {<n>}
pdbSet <material> ICluster Ifc   {<n>}
pdbSet <material> ICluster Isfc  {<n>}
pdbSet <material> ICluster Icf   {<n>}
pdbSet <material> ICluster Icr   {<n>}
pdbSet <material> ICluster Ikfcii {<n>}
pdbSet <material> ICluster Vkrv  {<n>}
pdbSet <material> ICluster Vrv   {<n>}
pdbSet <material> ICluster Vsrv  {<n>}
pdbSet <material> ICluster Vcrv  {<n>}
pdbSet <material> ICluster Vkfv  {<n>}
pdbSet <material> ICluster Vsfv  {<n>}
pdbSet <material> ICluster Vcfv  {<n>}

```

The changes are accompanied by corresponding inverse changes in  $C_I$ . Therefore, clustering reduces the number of free interstitials, while the dissolution of clusters releases interstitials.

Table 37 Solution names for 1Moment model of interstitials

Symbol	Solution name
$C_{ICluster}$	ICluster

## Vacancy

If you set the model to 1Moment, the model for the formation and dissolution of vacancy clusters or voids is included. The 1Moment model uses a single equation to calculate the total number of vacancies bound in clusters.

The following nonlinear algebraic equation along with the related diffusion equations are solved:

$$\frac{\partial C_{VCcluster}}{\partial t} = R_{CV} - R_{CI} \quad (577)$$

where  $C_{VCcluster}$  is the concentration of clustered vacancies, and  $R_{CV}$  and  $R_{CI}$  describe cluster interaction with vacancies and interstitials, respectively.

## 4: Diffusion

### Defect Clusters

The vacancy interaction includes two terms describing the clustering of vacancies and one describing the declustering:

$$R_{CV} = V_{kfi} \frac{(C_V)^{V_{fi}}}{(C_V^*)^{V_{sfi}}} + V_{kfc} \frac{(C_V)^{V_{fc}}}{(C_V^*)^{V_{sfc}}} (C_{VCluster} + V_{kfc} C_V) - V_{kr} (C_{VCluster})^{V_{cr}} \quad (578)$$

where  $C_V$  is the concentration of unclustered vacancies, and  $C_V^*$  is the equilibrium concentration of vacancies. The first term models nucleation of the vacancy clusters at high vacancy supersaturation. The second term models growth of the vacancy clusters by consuming free vacancies. The third term models dissolution of the vacancy clusters by emitting vacancies.

If the 1Moment model is used with the Full cluster model, Eq. 578 is modified as follows:

$$R_{CV} = (max + 1) R_{sVcl(max+1)} + V_{kfc} \frac{(C_V)^{V_{fc}}}{(C_V^*)^{V_{sfc}}} (C_{VCluster} + V_{kfc} C_V) - V_{kr} (C_{VCluster})^{V_{cr}} \quad (579)$$

where  $R_{sVcl(max+1)}$  is given in [Defect Cluster Model: Full on page 332](#). The smallest large-cluster forms when the small cluster captures one free vacancy by the reaction rate  $R_{sVcl(max+1)}$ .

The interstitial interaction includes one recombination and one generation term:

$$R_{CI} = I_{krv} \frac{(C_I)^{I_{rv}}}{(C_I^*)^{I_{srv}}} (C_{VCluster})^{I_{crv}} - I_{kf} (C_I^*)^{I_{sfv}} (C_{VCluster})^{I_{cfv}} \quad (580)$$

where  $C_I$  is the concentration of free interstitials, and  $C_I^*$  is the equilibrium concentration of interstitials. The first term models dissolution of the vacancy clusters by consuming interstitials. The second term models the emission of interstitials by the vacancy clusters.

To modify the dissolution rates  $V_{kr}$  and  $I_{kf}$  by complex prefactors, you can define the following terms in the command file:

```
term name= VClusterDissVacFactor silicon add eqn= {equation} store
term name= VClusterDissIntFactor silicon add eqn= {equation} store
```

If the 1Moment model is used with the Full cluster model, Eq. 580 is modified as follows:

$$R_{CI} = (max + 1) R_{sVcl(max+1)} + I_{krv} \frac{(C_I)^{I_{rv}}}{(C_I^*)^{I_{srv}}} (C_{VCluster})^{I_{crv}} - I_{kf} (C_I^*)^{I_{sfv}} (C_{VCluster})^{I_{cfv}} \quad (581)$$

where  $R_{sVcl(max+1)}$  is given in [Defect Cluster Model: Full on page 332](#). It is the reaction rate of small vacancy clusters with interstitials.

The reaction constants of the model can be modified using the following commands:

```

pdbSet <material> VCluster Vkfi  {<n>}
pdbSet <material> VCluster Vkfc  {<n>}
pdbSet <material> VCluster Vkr   {<n>}
pdbSet <material> VCluster Vfi   {<n>}
pdbSet <material> VCluster Vsfi  {<n>}
pdbSet <material> VCluster Vfc   {<n>}
pdbSet <material> VCluster Vsfc  {<n>}
pdbSet <material> VCluster Vcf   {<n>}
pdbSet <material> VCluster Vcr   {<n>}
pdbSet <material> VCluster Vkfci {<n>}
pdbSet <material> VCluster Ikrv  {<n>}
pdbSet <material> VCluster Irv   {<n>}
pdbSet <material> VCluster Isrv  {<n>}
pdbSet <material> VCluster Icrv  {<n>}
pdbSet <material> VCluster Ikfv  {<n>}
pdbSet <material> VCluster Isfv  {<n>}
pdbSet <material> VCluster Icfv  {<n>}

```

The changes are accompanied by corresponding inverse changes in  $C_V$ . Therefore, clustering reduces the number of free vacancies; while the dissolution of clusters releases vacancies.

Table 38 Solution names for 1Moment model for vacancies

Symbol	Solution name
$C_{V\text{Cluster}}$	VCluster

## Initializing 1Moment Model

The initial concentration of interstitial clusters or vacancy clusters after implantation is set in the `diffPreProcess` procedure (see [Ion Implantation to Diffusion on page 339](#)) and can be changed using the parameter `InitPercent` as follows:

```

pdbSet <material> ICcluster InitPercent {<n>}
pdbSet <material> VCluster InitPercent {<n>}

```

`InitPercent` is the percentage of free implantation interstitials used to initialize the model, for example:

$$ICcluster = \begin{cases} \text{Int\_Implant} * \text{InitPercent} & \text{Crystalline regions} \\ 0 & \text{Amorphous regions} \end{cases} \quad (582)$$

$$VCluster = \begin{cases} \text{Vac\_Implant} * \text{InitPercent} & \text{Crystalline regions} \\ 0 & \text{Amorphous regions} \end{cases} \quad (583)$$

The value of `InitPercent` must be between 0 and 1. The model assumes that existing interstitial or vacancy clusters in the amorphized region break apart.

---

## Defect Cluster Model: 2Moment

### Interstitial

If you set the model to `2Moment`, the model for the formation and dissolution of interstitial clusters (`{311}` or `{113}` defects) and conversion of `{311}` clusters into dislocation loops are included [42]. The model calculates the first two moments of the size distribution of interstitial clusters, in other words, the number of clusters and the number of interstitials contained in the clusters. It can be used with the existing model for dislocation loops (`LoopEvolution`), although it is designed to include modeling of at least some dislocation loops.

The `2Moment` clustering model is an implementation of the Gencer analytic kinetic precipitation model (AKPM). The density of clusters ( $D_{311}$ ) and concentration of interstitials ( $C_{311}$ ) contained in clusters are calculated as:

$$\frac{\partial D_{311}}{\partial t} = D_I \lambda_0 (C_I^2 - D_{311} C_{Ii}^* C_s \gamma_0) \quad (584)$$

$$\frac{\partial C_{311}}{\partial t} = 2 \frac{\partial D_{311}}{\partial t} + D_I \lambda_1 D_{311} (C_I - C_s C_{Ii}^* \gamma_1) \quad (585)$$

where  $C_I$  and  $D_I$  are the concentration and diffusivity of free interstitials. If the `2Moment` model is used with the `Full` cluster model, Eq. 584 and Eq. 585 are modified as follows:

$$\frac{\partial D_{311}}{\partial t} = R_{sIcl(max+1)} - R_{sIcV(max+1)} - D_I \lambda_0 D_{311} C_{Ii}^* C_s \gamma_0 \quad (586)$$

$$\frac{\partial C_{311}}{\partial t} = (max+1)(R_{sIcl(max+1)} - R_{sIcV(max+1)}) + D_I \lambda_1 D_{311} (C_I - C_s C_{Ii}^* \gamma_1) \quad (587)$$

$C_s \gamma_0$ , which gives the dependence of the dissolution rate on the average cluster size, is given by:

$$C_s \gamma_0 = \begin{cases} C_{ss} \frac{K_1}{s-1} & s < n_{crit} \\ C_{sl} K_3 \left( \frac{1}{s-1} \right)^\alpha & s > n_{crit} \end{cases} \quad (588)$$

where:

- $K_1$  controls the dissolution of two atom clusters.
- $s = C_{311}/D_{311}$  is the average number of interstitials in a cluster.

$C_s\gamma_1$ , which gives the dependence of the rate of interstitial release on the average cluster size, is given by:

$$C_s\gamma_1 = \begin{cases} C_{ss}\frac{s-2}{s+K_0}\left[1 + \frac{(K_0+2)K_2}{s+K_0}\right] & s < n_{crit} \\ C_{sl}\left[1 + K_4\left(\frac{K_0+2}{s+K_0}\right)^\alpha\right] & s > n_{crit} \end{cases} \quad (589)$$

where  $K_3$  and  $K_4$  are chosen to make  $C_s\gamma_0$  and  $C_s\gamma_1$  continuous at  $s = n_{crit}$ .  $C_{ss}, C_{sl}$  are the solid solubility of smaller and larger clusters.

To modify  $C_s\gamma_0$  and  $C_s\gamma_1$  by complex prefactors, you can define the following terms in the command file:

```
term name= C311DissIntFactor silicon add eqn= {equation} store
```

To set the model parameters, use the following commands:

```
pdbSet <material> C311 Lambda0      {<n>}
pdbSet <material> C311 Lambda1      {<n>}
pdbSet <material> C311 K0          {<n>}
pdbSet <material> C311 K1          {<n>}
pdbSet <material> C311 K2          {<n>}
pdbSet <material> C311 Alpha        {<n>}
pdbSet <material> C311 NCritical    {<n>}
pdbSet <material> Int SolubilitySmall {<n>}
pdbSet <material> Int SolubilityLarge {<n>}
```

[Eq. 584](#) models the nucleation and dissolution of two-atom clusters.  $\lambda_0$  is the capture length for these processes.

[Eq. 585](#) models the absorption and release of interstitials by clusters. The three terms on the right side model the absorption of interstitials during nucleation, the absorption of interstitials by nucleated clusters, and the release of interstitials by nucleated clusters.  $\lambda_1$  is the capture length for absorption and release of interstitials by nucleated clusters.  $C_{Ii}^*C_{ss}$  is the concentration of interstitials in equilibrium with a population of large {311} clusters.

For  $s > n_{crit}$ , some {311} defects unfault to form dislocation loops. These dislocation loops are included in the 2Moment model by modifying the cluster dissolution rates.  $\alpha$  controls the dissolution rate when loops are present, and  $C_{Ii}^*C_{sl}$  is the concentration of interstitials in equilibrium with a population of large dislocation loops,  $C_{Ii}C_{sl}$ .

#### 4: Diffusion

Defect Clusters

Table 39 Solution names for 2Moment model of interstitials

Symbol	Solution name
$C_{311}$	C311
$D_{311}$	D311

## Vacancy

If you set the model to 2Moment – the model for the formation and dissolution of vacancy clusters – the model calculates the first two moments of the size distribution of vacancy clusters, that is, the number of clusters and the number of vacancies contained in the clusters.

The 2Moment clustering model is an implementation of the Gencer analytic kinetic precipitation model (AKPM). The density of clusters ( $D_{void}$ ) and concentration of vacancies ( $C_{void}$ ) contained in clusters are calculated as:

$$\frac{\partial D_{void}}{\partial t} = D_V \lambda_0 (C_V^2 - D_{void} C_{Vi}^* C_s \gamma_0) \quad (590)$$

$$\frac{\partial C_{void}}{\partial t} = 2 \frac{\partial D_{void}}{\partial t} + D_V \lambda_1 D_{void} (C_V - C_s C_{Vi}^* \gamma_1) \quad (591)$$

where  $C_V$  and  $D_V$  are the concentration and diffusivity of free vacancies.

If the 2Moment model is used with the Full cluster model, Eq. 590 and Eq. 591 are modified as follows:

$$\frac{\partial D_{void}}{\partial t} = R_{sVcl(max+1)} - R_{sVcI(max+1)} - D_V \lambda_0 D_{void} C_{Vi}^* C_s \gamma_0 \quad (592)$$

$$\frac{\partial C_{void}}{\partial t} = (max+1)(R_{sVcl(max+1)} - R_{sVcI(max+1)}) + D_V \lambda_1 D_{void} (C_V - C_s C_{Vi}^* \gamma_1) \quad (593)$$

$C_s \gamma_0$ , which gives the dependence of the dissolution rate on the average cluster size, is given by:

$$C_s \gamma_0 = C_{ss} \frac{K_1}{s-1} \quad (594)$$

where:

- $K_1$  controls the dissolution of two atom clusters.
- $s = C_{void}/D_{void}$  is the average number of vacancies in a cluster.

$C_s\gamma_1$ , which gives the dependence of the rate of vacancy release on the average cluster size, is given by:

$$C_s\gamma_1 = C_{ss} \frac{s-2}{s+K_0} \left[ 1 + \frac{(K_0+2)K_2}{s+K_0} \right] \quad (595)$$

$C_{ss}$  are the solid solubility of clusters.

To modify  $C_s\gamma_0$  and  $C_s\gamma_1$  by complex prefactors, you can define the following terms in the command file:

```
term name= CVoidDissVacFactor silicon add egn= {equation} store
```

To set the model parameters, use the following commands:

```
pdbSet <material> CVoid Lambda0      {<n>}
pdbSet <material> CVoid Lambda1      {<n>}
pdbSet <material> CVoid K0           {<n>}
pdbSet <material> CVoid K1           {<n>}
pdbSet <material> CVoid K2           {<n>}
pdbSet <material> Vac SolubilitySmall {<n>}
```

[Eq. 590](#) models the formation and dissolution of di-vacancy clusters.  $\lambda_0$  is the capture length for these processes.

[Eq. 591](#) models the absorption and release of vacancies by clusters. The three terms on the right side model the absorption of vacancies during di-vacancy cluster formation, the absorption of vacancies by clusters, and the release of vacancies by clusters.  $\lambda_1$  is the capture length for absorption and release of vacancies by clusters.  $C_{Vi}^*C_{ss}$  is the concentration of vacancies in equilibrium with a population of large vacancy clusters.

Table 40 Solution names for 2Moment model of vacancies

Symbol	Solution name
$C_{void}$	CVoid
$D_{void}$	DVoid

## Initializing 2Moment Model

The initial concentration of interstitial clusters after implantation is set in the `diffPreProcess` procedure (see [Ion Implantation to Diffusion on page 339](#)). By default, clusters are assumed to break apart in the amorphous regions.

## 4: Diffusion

### Defect Clusters

You can specify the percentage of clusters retained in the amorphous region per cluster solution variable using the parameter `AmPercent`:

```

pdbSet <material> C311 AmPercent {<n>}
pdbSet <material> D311 AmPercent {<n>}

pdbSet <material> CVoid AmPercent {<n>}
pdbSet <material> DVoid AmPercent {<n>}

```

For example:

$$D_{311} = \begin{cases} D_{311} * \text{AmPercent} & \text{Amorphous regions} \\ D_{311} & \text{Crystalline regions} \end{cases} \quad (596)$$

The value of the `AmPercent` parameter must be between 0 and 1.

## Defect Cluster Model: Full

### Interstitial

If you set the defect cluster model to `Full`, the TS4 style transient small interstitial cluster model is used. The reactions associated with the size-n small interstitial cluster is as follows:



$I_n$  denote the n-size interstitial small cluster;  $I, V$  are the interstitials and vacancies. The transient equation for the n-size small interstitial cluster is:

$$\frac{\partial C_n}{\partial t} = R_{cI(n)} - R_{cV(n)} \quad 2 \leq n < n_{max} \quad (601)$$

$n_{max}$  can be set using the following command:

```
pdbSet Si Int CL.Size {<n>}
```

$R_{cI(n)}$  and  $R_{cV(n)}$  are described as follows:

$$R_{cI(n)} = R_{cI((n-1) \rightarrow (n))} - R_{cI((n) \rightarrow (n+1))} \quad (602)$$

$$R_{cV(n)} = R_{cV((n) \rightarrow (n-1))} - R_{cV((n+1) \rightarrow (n))} \quad (603)$$

$$R_{cI((n-1) \rightarrow (n))} = k_{fi}^{(n)} C_{I(n-1)} \frac{C_I}{C_I^*} - k_{ri}^{(n)} C_{I(n)} \quad (604)$$

$$R_{cI((n) \rightarrow (n+1))} = k_{fi}^{(n+1)} C_{I(n)} \frac{C_I}{C_I^*} - k_{ri}^{(n+1)} C_{I(n+1)} \quad (605)$$

$$R_{cV((n) \rightarrow (n-1))} = k_{rv}^{(n)} C_{I(n)} \frac{C_V}{C_V^*} - k_{fv}^{(n)} C_{I(n-1)} \quad (606)$$

$$R_{cV((n+1) \rightarrow (n))} = k_{rv}^{(n+1)} C_{I(n+1)} \frac{C_V}{C_V^*} - k_{fv}^{(n+1)} C_{I(n)} \quad (607)$$

here:

$$k_{fi}^{(n)} = C_{Ii}^* \sum_z f_{nz}^i k_{Iz} \left(\frac{n}{n_i}\right)^{-z} \quad n > 2 \quad (608)$$

$$k_{fi}^{(2)} = \frac{C_{Ii}^{*2}}{C_I^*} \sum_{z, q} f_{2qz}^i k_{Iz} k_{Iq} \left(\frac{n}{n_i}\right)^{-(z+q)} \quad n = 2 \quad (609)$$

$$k_{ri}^{(n)} = C_{Ii}^* \sum_z r_{nz}^i k_{Iz} \left(\frac{n}{n_i}\right)^{-z} \quad n > 2 \quad (610)$$

$$k_{ri}^{(2)} = C_{Ii}^* \sum_{z, q} r_{2qz}^i k_{Iz} k_{Iq} \left(\frac{n}{n_i}\right)^{-(z+q)} \quad n = 2 \quad (611)$$

$$k_{fv}^{(n)} = C_{Vi}^* \sum_z f_{nz}^v k_{Vz} \left(\frac{n}{n_i}\right)^{-z} \quad n > 2 \quad (612)$$

$$k_{fv}^{(2)} = \frac{C_{Ii}^* C_{Vi}^*}{C_I^*} \sum_z f_{2z}^v k_{Vz} \left(\frac{n}{n_i}\right)^{-z} \quad n = 2 \quad (613)$$

$$k_{rv}^{(n)} = C_{Vi}^* \sum_z r_{nz}^v k_{Vz} \left(\frac{n}{n_i}\right)^{-z} \quad (614)$$

## 4: Diffusion

### Defect Clusters

To set the reaction rate constants,  $f^i = k_{fi}$ ,  $f^v = k_{fv}$ ,  $r^i = k_{ri}$ ,  $r^v = k_{rv}$ , use:

```

pdbSet Si I2 kfI {<i,j>} {<n>}
pdbSet Si I2 krI {<i,j>} {<n>}
pdbSet Si I2 kfV {<i>} {<n>}
pdbSet Si I2 krV {<i>} {<n>}
pdbSet Si I3 kfI {<i>} {<n>}
pdbSet Si I3 krI {<i>} {<n>}
pdbSet Si I3 kfV {<i>} {<n>}
pdbSet Si I3 krV {<i>} {<n>}
pdbSet Si I4 kfI {<i>} {<n>}
pdbSet Si I4 krI {<i>} {<n>}
pdbSet Si I4 kfV {<i>} {<n>}
pdbSet Si I4 krV {<i>} {<n>}
pdbSet Si I5 kfI {<i>} {<n>}

```

The indices  $i$  and  $j$  are integers representing the charge state of interstitials and reacting interstitials. The shorthand `pdbSet` command can be used for clusters up to size 5. For all other clusters, the longhand `pdbSetDoubleArray` command must be used.

**NOTE** The indices for the parameters `kfI` and `krI` for  $I_2$  clusters have the form  $i, j$ . The indices are separated by a comma; no space is allowed between the indices.

If you want to use same reaction rate constants for all charges, use:

```
pdbSet Si Int CL.All <1 | 0>
```

If `CL.ALL` is set to 1, the model uses the 0th indexed reaction rate constants (for example, `kfI(0, 0)` or `kfI(0)`, `krV(0)` and so on) in the reaction calculation for all charge states.

To modify  $k_{ri}$  and  $k_{fv}$  by complex prefactors, you can define the following terms in the command file, for example, for  $I_2$ :

```

term name= I2DissIntFactor silicon add eqn= {equation} store
term name= I2DissVacFactor silicon add eqn= {equation} store

```

The net capture rate of free interstitials by the small interstitial clusters is given by:

$$R_{sIcl} = R_{cl(1 \rightarrow 2)} + \sum_{n=1}^{max} R_{cl(n \rightarrow n+1)} \quad (615)$$

The net capture rate of free vacancies by the small interstitial clusters is given by:

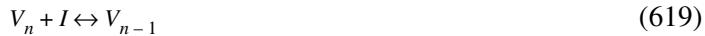
$$R_{sIcV} = \sum_{n=1}^{max} R_{cV(n \rightarrow n+1)} \quad (616)$$

Table 41 Solution names for full model of interstitials

Symbol	Solution name
$C_{I_2}$	I2
$C_{I_3}$	I3
$C_{I_4}$	I4
$C_{I_5}$	I5

## Vacancy

If you set the defect cluster model to Full, the TSUPREM-4-style transient small-vacancy cluster model is used. The reactions associated with the  $n$ -size small interstitial cluster are:



where  $V_n$  denotes the  $n$ -size small vacancy cluster, and  $I, V$  are the interstitials and vacancies.

The transient equation for the  $n$ -size small vacancy cluster is:

$$\frac{\partial C_n}{\partial t} = R_{cV(n)} - R_{cI(n)} \quad 2 \leq n < n_{max} \quad (621)$$

$n_{max}$  can be set using:

```
pdbsSet Si Vac CL.Size {<n>}
```

$R_{cV(n)}$  and  $R_{cI(n)}$  are described as follows:

$$R_{cV(n)} = R_{cV((n-1) \rightarrow (n))} - R_{cV((n) \rightarrow (n+1))} \quad (622)$$

$$R_{cI(n)} = R_{cI((n) \rightarrow (n-1))} - R_{cI((n+1) \rightarrow (n))} \quad (623)$$

$$R_{cV((n-1) \rightarrow (n))} = k_{fv}^{(n)} C_{V(n-1)} \frac{C_V}{C_V^*} - k_{rv}^{(n)} C_{v(n)} \quad (624)$$

#### 4: Diffusion

Defect Clusters

$$R_{cV((n) \rightarrow (n+1))} = k_{fv}^{(n+1)} C_{V(n)} \frac{C_V}{C_V^*} - k_{rv}^{(n+1)} C_{V(n+1)} \quad (625)$$

$$R_{cI((n) \rightarrow (n-1))} = k_{ri}^{(n)} C_{V(n)} \frac{C_I}{C_I^*} - k_{fi}^{(n)} C_{V(n-1)} \quad (626)$$

$$R_{cI((n+1) \rightarrow (n))} = k_{ri}^{(n+1)} C_{V(n+1)} \frac{C_I}{C_I^*} - k_{fi}^{(n+1)} C_{V(n)} \quad (627)$$

here:

$$k_{fv}^{(n)} = C_{Vi}^* \sum_z f_{nz}^i k_{Vz} \left(\frac{n}{n_i}\right)^{-z} \quad n > 2 \quad (628)$$

$$k_{fv}^{(2)} = \frac{C_{Vi}^{*2}}{C_{Vz,q}^*} \sum_z f_{2qz}^i k_{Vz} k_{Vq} \left(\frac{n}{n_i}\right)^{-(z+q)} \quad n = 2 \quad (629)$$

$$k_{rv}^{(n)} = C_{Vi}^* \sum_z r_{nz}^i k_{Vz} \left(\frac{n}{n_i}\right)^{-z} \quad n > 2 \quad (630)$$

$$k_{rv}^{(2)} = C_{Vi}^* \sum_{z,q} r_{2qz}^i k_{Vz} k_{Vq} \left(\frac{n}{n_i}\right)^{-(z+q)} \quad n = 2 \quad (631)$$

$$k_{fi}^{(n)} = C_{Ii}^* \sum_z f_{nz}^i k_{Iz} \left(\frac{n}{n_i}\right)^{-z} \quad n > 2 \quad (632)$$

$$k_{fi}^{(2)} = \frac{C_{Ii}^* C_{Vi}^*}{C_V^*} \sum_z f_{2z}^i k_{Iz} \left(\frac{n}{n_i}\right)^{-z} \quad n = 2 \quad (633)$$

$$k_{ri}^{(n)} = C_{Ii}^* \sum_z r_{nz}^i k_{Iz} \left(\frac{n}{n_i}\right)^{-z} \quad (634)$$

To set the reaction rate constants,  $f^v = k_{fv}$ ,  $f^i = k_{fi}$ ,  $r^v = k_{rv}$ ,  $r^i = k_{ri}$ , use:

```

pdbSet Si V2 kfV {<i,j>} {<n>}
pdbSet Si V2 krV {<i,j>} {<n>}
pdbSet Si V2 kfI {<i>} {<n>}
pdbSet Si V2 krI {<i>} {<n>}
pdbSet Si V3 kfV {<i>} {<n>}
pdbSet Si V3 krV {<i>} {<n>}

```

```

pdbSet Si V3 kfI {<i>} {<n>}
pdbSet Si V3 krI {<i>} {<n>}
pdbSet Si V4 kfV {<i>} {<n>}
pdbSet Si V4 krV {<i>} {<n>}
pdbSet Si V4 kfI {<i>} {<n>}
pdbSet Si V4 krI {<i>} {<n>}
pdbSet Si V5 kfV {<i>} {<n>}
pdbSet Si V5 krV {<i>} {<n>}
pdbSet Si V5 kfI {<i>} {<n>}
pdbSet Si V5 krI {<i>} {<n>}
pdbSet Si V6 kfV {<i>} {<n>}
pdbSet Si V6 krV {<i>} {<n>}
pdbSet Si V6 kfI {<i>} {<n>}
pdbSet Si V6 krI {<i>} {<n>}
pdbSet Si V7 kfV {<i>} {<n>}
pdbSet Si V7 krV {<i>} {<n>}
pdbSet Si V7 kfI {<i>} {<n>}
pdbSet Si V7 krI {<i>} {<n>}
pdbSet Si V8 kfV {<i>} {<n>}

```

The indices  $i$  and  $j$  are integers representing the charge state of vacancies and reacting vacancies. The shorthand `pdbSet` command can be used for clusters up to size 8. For all other clusters, the longhand `pdbSetDoubleArray` command must be used.

**NOTE** The indices for the parameters `kfV` and `krV` for  $V_2$  clusters have the form of  $i, j$ . The indices are separated by a comma; no space is allowed between the indices.

If you want to use same reaction rate constants for all charges, use:

```
pdbSet Si Vac CL.All <1 | 0>
```

If `CL.ALL` is set to 1, the model uses the 0th indexed reaction rate constants (for example, `kfV(0, 0)` or `krI(0)` and so on) in the reaction calculation for all charge states.

To modify  $k_{rv}$  and  $k_{fi}$  by complex prefactors, you can define the following terms in the command file, for example, for  $V_2$ :

```

term name= V2DissVacFactor silicon add eqn= {equation} store
term name= V2DissIntFactor silicon add eqn= {equation} store

```

The net capture rate of free vacancies by the small vacancy clusters is given by:

$$R_{sVcl} = R_{cV(1 \rightarrow 2)} + \sum_{n=1}^{\max} R_{cV(n \rightarrow n+1)} \quad (635)$$

The net capture rate of free interstitials by the small vacancy clusters is given by:

$$R_{sVcI} = \sum_{n=1}^{\max} R_{cI(n \rightarrow n+1)} \quad (636)$$

Table 42 Solution names for full model of vacancies

Symbol	Solution name
$C_{V_2}$	V2
$C_{V_3}$	V3
$C_{V_4}$	V4
$C_{V_5}$	V5
$C_{V_6}$	V6
$C_{V_7}$	V7
$C_{V_8}$	V8

## Initializing Full Model

The initial concentration of interstitial or vacancy clusters after implantation is set in the `diffPreProcess` procedure (see [Ion Implantation to Diffusion on page 339](#)). By default, clusters are assumed to break apart in the amorphous regions. You can specify the percentage of clusters retained in the amorphous region per cluster solution variable using the parameter `AmPercent`:

```
pdbSet <material> <cluster> AmPercent {<n>}
```

For example:

$$I_4 = \begin{cases} I_4 * \text{AmPercent} & \text{Amorphous regions} \\ I_4 & \text{Crystalline regions} \end{cases} \quad (637)$$

The value of the `AmPercent` parameter must be between 0 and 1.

In addition, you can specify the initial concentration of interstitial or vacancy clusters after implantations by using the parameter `InitPercent` as follows:

```
pdbSet <material> <cluster> InitPercent {<n>}
```

The parameter `InitPercent` is the percentage of free implantation interstitials or vacancies used to initialize the model, for example:

$$ICluster = \begin{cases} \text{Int\_Implant} * \text{InitPercent} & \text{Crystalline regions} \\ 0 & \text{Amorphous regions} \end{cases} \quad (638)$$

The value of `InitPercent` must be between 0 and 1.

## Ion Implantation to Diffusion

During implantation, important data fields (see [Chapter 3 on page 53](#)) such as `Int_Implant`, `Vac_Implant`, and `Damage` are created.

`Int_Implant` and `Vac_Implant` represent the total number of interstitial and vacancy point-defects coming from the ion implantation. Since it is possible that the point defects already exist in the structure or amorphization occurred due to ion implantation, the point-defect fields must be updated before any diffusion step.

Sentaurus Process calls a default procedure, `diffPreProcess`, to process these fields. The main goal of the procedure is to process the point-defect fields and to store the processed fields in the `Interstitial` and `Vacancy` data fields. These data fields represent the total number of interstitials and vacancies that will be used to initialize the total number of unpaired interstitials (`Int`) and vacancies (`Vac`) (see [Initializing Solution Variables on page 342](#)):

$$\text{Interstitial} = \begin{cases} \text{Interstitial} + \text{Int\_Implant} & \text{Crystalline regions} \\ C_I^* & \text{Amorphous regions} \end{cases} \quad (639)$$

$$\text{Vacancy} = \begin{cases} \text{Vacancy} + \text{Vacancy\_Implant} & \text{Crystalline regions} \\ C_V^* & \text{Amorphous regions} \end{cases} \quad (640)$$

First, interstitials and vacancies from implantations (`Int_Implant`, `Vac_Implant`) are added to existing `Interstitial` and `Vacancy` fields in the crystalline regions. If the fields do not exist, they are created and set to their equilibrium values.

The `Damage` field is used to determine whether the material is amorphized. The threshold value for the amorphization can be set by:

```
pdbSet <material> AmorpDensity {<n>}
```

It is assumed that if a material amorphizes due to ion implantation, the amorphized portion of the material will grow to a perfect crystalline material and point-defect densities in this region will be equal to their thermal equilibrium values (see [Eq. 640](#)). If a material is an amorphized

## 4: Diffusion

### Ion Implantation to Diffusion

material (that is, polysilicon), the point-defect densities in this material are set automatically to their equilibrium values.

The abovementioned amorphization algorithm leads to very steep interstitial profiles at the amorphous–crystalline boundary. This boundary can be softened using an error function. The degree of smoothing can be controlled using the parameter `AmorpGamma`, that is:

```
pdbSet <material> AmorpGamma {<n>}
```

The value of this parameter must be between 0 and 1, where 1 means a very steep transition. Smoothing also will be applied to dopant profiles if the transient or cluster model is selected. To find out whether a material is amorphous, use the commands:

```
pdbGet <material> Amorphous  
pdbSet <material> Amorphous 1 or 0
```

When the point-defect concentrations are set to their equilibrium values in the amorphous regions, their densities in non-amorphous regions are compared to the solid solubility values of these defects in each material. If the solid solubility values are defined, the defect profiles are cut off at the solid solubility values. To specify the solid solubility numbers for the `Interstitial` and `Vacancy` fields, use:

```
pdbSet <material> Int TotSolubility {<n>}  
pdbSet <material> Vac TotSolubility {<n>}  
  
Interstitial = min(Interstitial, InfTotSolubility) (641)  
Vacancy = min(Vacancy, VacTotSolubility)
```

In addition to the processing of implantation data fields, the `diffPreProcess` procedure determines whether point-defect equations need to be solved. As a default behavior, Sentaurus Process does not solve the defect equations if the dopant diffusion models are set to `Fermi` (see [Fermi Diffusion Model on page 190](#)), or `Constant` (see [Constant Diffusion Model on page 191](#)), or `ChargedFermi` (see [ChargedFermi Diffusion Model on page 188](#)) in all materials with the following exceptions:

- Both point-defect equations are switched on if the point-defect clusters are switched on.
- Only the interstitial point-defect equation is switched on during oxidation unless the point-defect clusters are switched on.

Both point-defect equations are solved if the dopant diffusion models are set to `Pair` (see [Pair Diffusion Model on page 187](#)), or `React` (see [React Diffusion Model on page 183](#)), `ChargedPair` (see [ChargedPair Diffusion Model on page 185](#)), or `ChargedReact` (see [ChargedReact Diffusion Model on page 176](#)) in any material.

Although it is not recommended, you may want to switch on or off the point-defect equations for any chosen dopant diffusion model. In this case, use the commands:

```
pdbSetBoolean Defect Int ForcedTurnOff 1
pdbSetBoolean Defect Vac ForcedTurnOff 1
pdbSetBoolean Defect Int ForcedTurnOn 1
pdbSetBoolean Defect Vac ForcedTurnOn 1
```

**NOTE** These parameters are not in the parameter database and are provided for advanced users.

To change the initialization of point defects in the amorphous regions, use:

```
pdbSet <material> Int Truncation.Model <model>
pdbSet <material> Vac Truncation.Model <model>
```

where `<model>` is either `None` or `Equilibrium`. The default is `None` and follows the initialization procedure previously explained in [Initializing Solution Variables on page 342](#).

The `Equilibrium` model sets the unpaired total interstitial (`Int`) and vacancy (`Vac`) concentrations to the user-defined equilibrium values,  $C_X^*$  (see [Eq. 142, p. 183](#)).

The `diffPreProcess` procedure also initializes the fluorine model (see [Initializing the FVCluster Model on page 293](#)), the active dopant models `Cluster` and `Transient` (see [Initializing Transient Model on page 284](#)), the {311} defect-clustering model (see [Initializing 311 Model on page 314](#)), and the 1Moment defect-clustering model (see [Initializing 1Moment Model on page 327](#)).

When the preprocessing of the data fields is completed, most implantation fields are deleted. Sentaurus Process also calls the `diffPostProcess` procedure as soon as diffusion has finished. In this procedure, remaining implantation fields are cleared and total defect concentrations are stored for use with the next `diffuse` command during initialization.

**NOTE** Every time that an implantation is followed by an annealing, the equilibrium concentration of a point defect is added to the concentration of the defect during initialization. Therefore, it may lead to an unexpected increase in the concentrations of the defects in the depth of the structure in some special cases. To resolve this, switch on the `Use.New.Init.Method` parameter:

```
pdbSet Diffuse Use.New.Init.Method 1
```

## Initializing Solution Variables

Initializing solution variables is typically a minor task in Sentaurus Process. You can manipulate data and easily modify any data field using the `select` command (see [select on page 1168](#)). Data fields can be added, subtracted, truncated, or manipulated in many ways.

You also can define special callback procedures to initialize solution variables in different ways. This section covers the callback procedures and the keywords used by Sentaurus Process to initialize solution variables.

No nonlinear or partial differential equations are solved to initialize dopant solutions. Dopant data fields generated during implantation are simply added to existing ones. For example, if you select the dopant diffusion model `React` (see [React Diffusion Model on page 183](#)), there is no contribution to the dopant–defect pair fields from the implantation. However, you can use the `select` command to distribute dopants among the other fields as required.

Conversely, Sentaurus Process uses callback procedures (see [Using Callback Procedures to Build Models on page 618](#)) to initialize the total number of unpaired interstitials (`Int`) and vacancies (`Vac`), which are used as solution names. Since extra dopant–defect equations are not solved for the `Pair`, `ChargedPair`, or `ChargedFermi` dopant diffusion models, transferring all point defects from implantation to their respective solution names may cause an artificial increase of dopant–defect pairs in the structure. To prevent this artificial dopant–defect pair increase, defects from implantation must be added to the total interstitials and vacancies.

The main callback procedures to initialize solution variables are `EquationInitProc` and `InitSolve`. To initialize a solution variable, the keyword `InitStep` must be defined with the solution variable. This is different from the typical use of callback procedures (see [Using Callback Procedures to Build Models on page 618](#)):

```
pdbSetString <material> <solution> InitSolve <callback procedure>
pdbSetString <material> <solution> EquationInitProc <callback procedure>
```

The procedures take three arguments: a material, a solution, and the name of the callback procedure. For example, the following command *informs* the code to invoke the `ResetInit` procedure every time that solutions are checked:

```
pdbSetString Si Int InitSolve ResetInit
```

This is usually performed at the very beginning of a diffusion step. The `ResetInit` procedure could be defined as:

```
fproc ResetInit { Mat Sol } {
    pdbUnSetString $Mat $Sol Equation
}
```

When a solution variable requires initialization, Sentaurus Process searches for whether the `EquationInitProc` callback procedure is used for the solution name. If it is used, Sentaurus Process executes the procedure given with the command. Otherwise, you must provide the initialization equation. The following command *informs* Sentaurus Process to call the procedure `InitializeInt` before parsing the initialization equation for the solution `Int`:

```
pdbSetString Si Int EquationInitProc InitializeInt
```

The `InitializeInt` procedure could be defined as:

```
fproc InitializeInit { Mat Sol } {
    pdbSetString $Mat $Sol Equation "$Sol - 1e17"
}
```

In this case, the initialization equation for the solution name `Int` will be set to `Int - 1e17 = 0`.

When the initialization is completed, `Int` will have the value of  $1 \times 10^{17}$  in the specified material. This is a trivial example, but you can define any valid equation in this procedure.

For example, the default initialization equation for `Int` in Sentaurus Process, which can change depending on the dopants and diffusion models, can be:

```
Interstitial - (Int + (I0 * BActive * (( [expr [Arrhenius 5.68 0.48] * \
[pdbGetDouble Si Boron Int Binding] ] + [expr 0.0 * \
[pdbGetDouble Si Boron Int Binding] ] * Noni) * Noni + ( \
[expr [Arrhenius 5.68 0.42] * [pdbGetDouble Si Boron Int Binding] ] + \
[expr 0.0 * [pdbGetDouble Si Boron Int Binding] ] * Poni) * Poni + \
([expr 1.0 * [pdbGetDouble Si Boron Int Binding] ])))) = 0
```

where `I0`, `BActive`, `Noni`, and `Poni` are a function of the solution `Int`.

**NOTE** The `InitPostProcess` procedure (see [Figure 75 on page 620](#)) can be used to save and plot solution variables after the initialization is completed.

## Boundary Conditions

Different boundary conditions can be selected in Sentaurus Process using:

```
pdbSet <interface_material> <dopant> | <defect> BoundaryCondition <model>
```

where:

- <interface\_material> is the name of an interface material (see [Specifying Materials on page 18](#)).
- <dopant> is the name of a dopant.

## 4: Diffusion

### Boundary Conditions

- <defect> is either Interstitial or Vacancy.
- <model> is one of the available models:
  - HomNeumann
  - Natural
  - Segregation
  - Dirichlet
  - ThreePhaseSegregation
  - Trap
  - TrapGen
  - Continuous

For example, the following command sets the Dirichlet boundary condition at the oxide–silicon interface for interstitials:

```
pdbSet Oxide_Silicon Int BoundaryCondition Dirichlet
```

---

## HomNeumann

It is assumed that there are no fluxes and transfers across the interface. This is chosen by default at the front, back, left, right, and bottom boundaries, and can be applied to any boundary.

---

## Natural

This is the default boundary condition for point defects at gas–silicon and oxide–silicon interfaces. The normal flux across an outer surface is given by:

$$\mathbf{j} \bullet \mathbf{n} = h(C - C^*) \quad (642)$$

where  $h$  is the surface recombination rate, and  $C$  and  $C^*$  are the concentration of interstitials or vacancies and equilibrium concentration of interstitials and vacancies, respectively. The equilibrium concentration of point defects at the surface can be modified using user-defined parameters (see [Modifying Point-Defect Equilibrium Values at Surface on page 347](#)). There are four surface recombination velocity models:

- PDependent
- InitGrowth

- Simple
- Normalized

To set the models, use:

```
pdbSet <interface material> <defect> Surf.Recomb.Vel <model>
```

where:

- <interface material> is an interface material name (see [Specifying Materials on page 18](#)).
- <defect> is either Interstitial or Vacancy.
- <model> is one of the model names.

In each case, the surface recombination rate depends on the motion of the interface due to oxidation.

## Surface Recombination Model: PDependent

The PDependent model is the pressure-dependent surface recombination model. The flux that takes into account the interstitial injection during oxidation is given by:

$$\mathbf{j} \bullet \mathbf{n} = k_s \left( 1 + k_{Rat} \left( \frac{\|V_{ox}\|}{V_{Scale}} \right)^{k_{pow}} P_o^{k_{ppow}} \right) (C_{X^0} - C_{X^0}^*) - G_{ox} \quad (643)$$

where:

- $k_s$  is the surface recombination rate.
- $G_{ox}$  is the generation rate.
- $P_o$  is the oxygen partial pressure.
- $\|V_{ox}\|$  is the local oxidation rate (ReactionSpeed).
- $V_{Scale}$  is the reference oxidation rate for bare, undoped silicon.
- $k_{Rat}$ ,  $k_{pow}$ , and  $k_{ppow}$  are model parameters.

To modify these parameters, use:

```
pdbSet <interface material> <defect> Ksurf {<n>}
pdbSet <interface material> <defect> Scale {<n>}
pdbSet <interface material> <defect> Krat {<n>}
pdbSet <interface material> <defect> Kpow {<n>}
pdbSet <interface material> <defect> Kppow {<n>}
```

## 4: Diffusion

### Boundary Conditions

The generation term,  $G_{ox}$ , is given by:

$$G_{ox} = \theta \|V_{ox}\| L_{den} \left( \frac{\|V_{ox}\|}{V_{Scale}} \right)^{G_{pow}} P_o^{G_{gpow}} G_{Scale} \quad (644)$$

$G_{pow}$ ,  $G_{gpow}$ , and  $\theta$  are model parameters to adjust the interstitial injection during oxidation.

To modify these parameters, use:

```
pdbSet <interface material> <defect> Gpow {<n>}
pdbSet <interface material> <defect> Ggpow {<n>}
pdbSet <interface material> <defect> theta {<n>}
```

$L_{den}$  is the lattice density of silicon and can be set by:

```
pdbSet <material> LatticeDensity {<n>}
```

$G_{Scale}$  is the scaling factor for the generation rate and given by:

$$G_{Scale} = \begin{cases} G_0 & G_{low} = 0 \text{ and Charged Model} \\ G_1 G_{low} & G_{low} \neq 0 \end{cases} \quad (645)$$

$$G_0 = \frac{C_{X_i}^*}{C_X^*} \quad (646)$$

$$G_1 = \frac{mm + m + 1 + p + pp}{mm\left(\frac{n}{n_i}\right)^{2PotOx} + m\left(\frac{n}{n_i}\right)^{PotOx} + 1 + p\left(\frac{p}{n_i}\right)^{PotOx} + pp\left(\frac{p}{n_i}\right)^{2PotOx}} \quad (647)$$

If the dopant diffusion model is set to ChargedFermi or ChargedPair or ChargedReact and  $G_{low}$  is zero,  $G_{Scale}$  will be set to  $G_0$ ; otherwise, it will be set to  $G_1$ .

$G_{low}$ ,  $PotOx$ ,  $mm$ ,  $m$ ,  $p$ , and  $pp$  are model parameters that can be modified with the commands:

```
pdbSet <interface material> <defect> PotOx {<n>}
pdbSet <interface material> <defect> mm {<n>}
pdbSet <interface material> <defect> m {<n>}
pdbSet <interface material> <defect> p {<n>}
pdbSet <interface material> <defect> pp {<n>}
pdbSet <interface material> <defect> Glow {<n>}
```

## Surface Recombination Model: InitGrowth

The **InitGrowth** model is almost identical to **PDependent** (see [Surface Recombination Model: PDependent on page 345](#)) except that  $\|V_{ox}\|/V_{Scale}$  is set to 1 for nonoxidizing cases in Eq. 643.

## Surface Recombination Model: Simple

The **Simple** model takes into account the interstitial injection through total free and equilibrium point-defect concentrations during oxidation. The recombination flux is given by:

$$\mathbf{j} \bullet \mathbf{n} = k_s \left( 1 + k_{Rat} \left( \frac{\|V_{ox}\|}{V_{Scale}} \right) \right) (C_X - C_X^*) - G_{ox} \quad (648)$$

$$G_{ox} = \theta \|V_{ox}\| L_{den} G_{Scale} \quad (649)$$

$G_{Scale}$  is given by [Eq. 645](#).

## Surface Recombination Model: Normalized

The **Normalized** model is a TSUPREM-4-type surface recombination model. This model provides both the time dependence and the dependence on the oxidation conditions by using a constant normalizing factor:

$$\mathbf{j} \bullet \mathbf{n} = \left( k_s + k_{svel} \left( \frac{\|V_{ox}\|}{V_{Scale}} \right)^{kpow} \right) (C_X - C_X^*) - G_{ox} \quad (650)$$

$$G_{ox} = \theta L_{den} \|V_{ox}\| \left( \frac{\|V_{ox}\|}{V_{Scale}} \right)^{G_{pow}} G_{Scale} \quad (651)$$

To set the normalizing factor, use:

```
pdbSet <interface material> <defect> Ksvel {<n>}
```

$G_{Scale}$  is given by [Eq. 645](#).

## Modifying Point-Defect Equilibrium Values at Surface

The equilibrium value of point defects at the interface can be enhanced as follows:

$$C_{X\ Enhanced}^* = C_X^* \left( 1 + F_{ox} G_1 \left( \frac{\|V_{ox}\|}{V_{ref}} \right)^{P_{ox}} \right) \quad (652)$$

$G_1$  is given by [Eq. 647](#).

$V_{ref}$ ,  $F_{ox}$ , and  $P_{ox}$  are model parameters that can be modified with the commands:

```
pdbSet <interface material> <defect> VrefRate {<n>}
pdbSet <interface material> <defect> Fox      {<n>}
pdbSet <interface material> <defect> Pox      {<n>}
```

To switch on the enhancement, use the command:

```
pdbSet <interface material> <defect> HybridBC {1 | 0}
```

## Segregation

This is the default boundary condition for dopants at all interfaces except for phosphorus at oxide–silicon, oxide–SiC, and oxynitride–silicon interfaces. The segregation boundary condition is also known as the two-phase segregation boundary condition. The total dopant fluxes at the interfaces are balanced. The fluxes are assumed to be proportional to the deviation from the segregation equilibrium. The fluxes are given by:

$$\mathbf{j} \bullet \mathbf{n} = h \left( C_A^a - \frac{C_A^b}{s} \right) \quad (653)$$

where:

- $C_A^a$  is the concentration of dopant on one side of the interface.
- $C_A^b$  is the concentration of dopant on the other side of the interface.
- $h$  is the transfer rate.
- $s$  is the segregation rate of dopant  $A$ .

If the charge states of the dopants must be included or the boundary condition for dopant–defect pairs must be set, use the command:

```
pdbSet <interface_material> <dopant> Surf.Recomb.Model <bulk_diffusion_model>
<model>
```

where:

- $<\text{interface\_material}>$  is the name of an interface material (see [Specifying Materials on page 18](#)).
- $<\text{dopant}>$  is a valid dopant name.

- `<bulk_diffusion_model>` is one of the following dopant diffusion models for `<dopant>` on either side of the interface: Constant, Fermi, ChargedFermi, Pair, ChargedPair, React, or ChargedReact.
- `<model>` is either Default or PairSegregation.

**NOTE** See [Dependency on Interface Crystal Orientation on page 359](#) for orientation-dependent segregation.

## Surface Recombination Model: Default

If the surface recombination model is set to Default for any dopant diffusion model, the segregation fluxes are given by:

$$\mathbf{j} \bullet \mathbf{n} = k_{Transfer} \left( C_A^a - \frac{C_A^b}{k_{Segregation}} \right) \quad (654)$$

To set these parameters, use the commands:

```
pdbSet <interface material> <dopant> Transfer {<n>}
pdbSet <interface material> <dopant> Segregation {<n>}
```

**NOTE** If the dopant diffusion model is set to React or ChargedReact,  $C_A$  will be the substitutional dopant.

Sentaurus Process allows these transfer rates and segregation rates to be multiplied by a user-defined term for individual dopants. For example, for the Transfer parameter, the value of  $k_{Transfer}$  will become:

$$k_{Transfer} = \text{TransferFactor} \times k_{Transfer} \quad (655)$$

These term factors must be defined as `<dopant>SegregationFactor` and `<dopant>TransferFactor`. For example, the factors for boron at the oxide–silicon interface can be defined as follows:

```
term name= <dopant>SegregationFactor add Oxide /Silicon eqn= "<expr>" store
term name= <dopant>TransferFactor add Oxide /Silicon eqn= "<expr>" store
```

## Surface Recombination Model: PairSegregation

If the surface recombination model is set to PairSegregation for the Constant, Fermi, ChargedFermi, Pair, or ChargedPair diffusion models, the segregation fluxes are given by:

$$\mathbf{j} \bullet \mathbf{n} = k_{Transfer} k_{rate}^a k_{rate}^b \left( C_A^a \left( \frac{n}{n_i} \right)_a^z - \frac{C_A^a \left( \frac{n}{n_i} \right)_a^z}{k_{Segregation}} \right) \quad (656)$$

$$k_{rate}^{a/b} = \left( f_I \left[ \frac{C_I^*}{C_I^*} \right]_{a/b}^{(1-\gamma_I)} + (1-f_I) \left[ \frac{C_V^*}{C_V^*} \right]_{a/b}^{(1-\gamma_V)} \right) \quad (657)$$

where:

- $f_I$  is the interstitial fraction of dopant trapping in equilibrium.
- $\gamma_I$  and  $\gamma_V$  are the parameters Scale.PairSegregation ( $0 \leq \gamma_I, \gamma_V \leq 1$ ) that control interstitial and vacancy injections, respectively.

To set these parameters, use:

```
pdbSet <interface material> <dopant> Trap.Fi {<n>}
pdbSet <interface material> <dopant> <defect> Scale.PairSegregation_${side}
{<n>}
```

To use the total unpaired interstitial concentration, instead of the neutral one, use:

```
pdbSet <interface material> <dopant> UseUnpairedTotalInt <1 | 0>
```

In this case, Eq. 657 will be:

$$k_{rate}^{a/b} = \left( f_I \left[ \frac{C_I^*}{C_I^*} \right]_{a/b}^{(1-\gamma_I)} + (1-f_I) \left[ \frac{C_V^*}{C_V^*} \right]_{a/b}^{(1-\gamma_V)} \right) \quad (658)$$

If the dopant diffusion model is not Pair or ChargedPair model on interface side  $a$ ,  $k_{rate}^a$  is set to 1. If the same is true for interface side  $b$ ,  $k_{rate}^b$  is set to 1.

If the surface recombination model is set to PairSegregation for React or ChargedReact diffusion models, the segregation fluxes are given by:

$$\mathbf{j} \bullet \mathbf{n} = k_{Transfer} k_{AIrate}^a \left[ C_I^* \left( \frac{n}{n_i} \right)_a^b C_A^a \left( \frac{n}{n_i} \right)_a^z - \frac{C_{AI}^b \left( \frac{n}{n_i} \right)_b^z}{k_{Segregation} \sum_z k_{AI}^b k_{Iz}^b \left( \frac{n}{n_i} \right)_b^{-z}} \right] \quad (659)$$

$$\mathbf{j} \bullet \mathbf{n} = k_{Transfer} k_{AVrate}^a \left[ [C_{V^0}^*]^b C_A^a \left( \frac{n}{n_i} \right)^z - \frac{C_{AV}^b \left( \frac{n}{n_i} \right)^z}{k_{Segregation} \sum_z k_{AV^z}^b k_{V^z}^b \left( \frac{n}{n_i} \right)^{-z}} \right] \quad (660)$$

$$k_{AIrate}^a = \frac{f_I}{[C_I^0]^b} k_{rate}^a \quad (661)$$

$$k_{AVrate}^a = \frac{1-f_I}{[C_{V^0}^*]^b} k_{rate}^a \quad (662)$$

where  $C_{AI}$  and  $C_{AV}$  are the concentration of dopant–defect pairs.  $C_A$  is the concentration of the total unpaired dopant.

To use the total unpaired interstitial and vacancy concentrations, Eq. 661 and Eq. 662 will be:

$$k_{AIrate}^a = \frac{f_I}{[C_I^0]^b} \frac{\sum_c k_f^c \left( \frac{n}{n_i} \right)^{-c}}{\sum_c k_f^s} k_{rate}^a \quad (663)$$

$$k_{AVrate}^a = \frac{1-f_I}{[C_{V^0}^*]^b} \frac{\sum_c k_{V^c}^c \left( \frac{n}{n_i} \right)^{-c}}{\sum_c k_{V^c}^s} k_{rate}^a \quad (664)$$

## Dirichlet

The Dirichlet boundary condition can be used with both point defects and dopants. However, it can be set only at gas and any other material interfaces for dopants. In this way, ‘in-diffusion’ for a dopant can be simulated using the Dirichlet boundary condition. If the Dirichlet boundary condition is selected, the defect or dopant concentration at the boundary is set to its equilibrium value. The equilibrium value can be specified with:

```
pdbSet <material> {<dopant> | <defect>} Cstar <n>
```

where:

- <material> is a material name.
- <dopant> is a valid dopant name.

## 4: Diffusion

### Boundary Conditions

- <defect> is either Interstitial or Vacancy.
- Cstar is the equilibrium value of the solution variable.

If the Dirichlet boundary condition is selected and the oxidation is switched on, the modified Dirichlet boundary condition is used for interstitials. The equilibrium value of interstitial point-defects at the interface is enhanced (see [Modifying Point-Defect Equilibrium Values at Surface on page 347](#)) and the new equilibrium at the interface becomes:

$$C_{I_{ox}}^* = C_{I_0}^* \left( 1 + F_{ox} G_1 \left( \frac{\|V_{ox}\|}{V_{ref}} \right)^{P_{ox}} \right) \quad (665)$$

---

## ThreePhaseSegregation

This is the default boundary condition for phosphorus at oxide–silicon, oxide–SiC, and oxynitride–silicon interfaces. Dose loss during diffusion can be modeled with three-phase segregation in Sentaurus Process. Dopants can segregate from both silicon and oxide to the silicon–oxide interface where they are considered inactive. The model in Sentaurus Process is based on the original model by Lau *et al.* [43], and Oh and Ward [44]. The diffusion equation at the interface is given by:

$$\frac{\partial C_A}{\partial t} = \nabla D_0 \nabla C_A + F_a + F_b \quad (666)$$

where  $D_0$  is the diffusivity of the dopant at the interface, and  $F_a$  and  $F_b$  are the flux towards the interface from material  $a$  and material  $b$ , respectively.

The diffusivity at the interface can be defined by:

```
pdbSet <interface material> <dopant> D <c> {<n>}
```

where:

- <interface material> is an interface material name (see [Specifying Materials on page 18](#)).
- <dopant> is one of the existing Sentaurus Process dopants.
- <c> is the charge state.
- <n> is a Tcl expression that returns a number; it can be simply a number.

**NOTE** Only a neutral charge state is considered at the interface.

The fluxes  $F_a$  and  $F_b$  depend on the surface recombination model used. The surface recombination models are Default or PairSegregation, and can be set for different diffusion models using the command:

```
pdbSet <interface_material> <dopant> Surf.Recomb.Model <bulk_diffusion_model>
      <model>
```

where:

- <interface material> is an interface material name (see [Specifying Materials on page 18](#)).
- <dopant> is the name of the dopant.
- <bulk\_diffusion\_model> is one of the following dopant diffusion models for <dopant> on either side of the interface: Constant, Fermi, ChargedFermi, Pair, ChargedPair, React, or ChargedReact.

For example, if the boron diffusion model is set to the Pair model on the silicon side of an interface and the Constant model is set on the oxide side, and Surf.Recomb.Model is set as follows:

```
pdbSet Oxide_Silicon Boron Surf.Recomb.Model {Constant {Default}
                                              Pair {PairSegregation}}
```

$F_a$  and  $F_b$  are calculated using the Default model and the PairSegregation model, respectively.

- <model> is either Default or PairSegregation.

**NOTE** See [Dependency on Interface Crystal Orientation on page 359](#) for orientation-dependent segregation.

## Surface Recombination Model: Default

If the surface recombination model is set to Default for any dopant diffusion model, the segregation fluxes are given by:

$$F_{a/b} = T_{Rate}^{a/b} \left( [C_A^{Tmax}]^{a/b} - \sum_i C_{A_i} \right) [C_A^+]^{a/b} \left( \frac{n}{n_t} \right)^z - E_{Rate}^{a/b} C_A \left( \frac{[C_A^{ss}]^{a/b} \cdot [C_A^{ss}]^{a/b}}{[C_A^{ss}]^{a/b} + [C_A^+]^{a/b}} \right) \quad (667)$$

where:

- $T_{Rate}$  is the trapping rate.
- $C_A^{Tmax}$  is the maximum number of sites in the adjacent bulk regions.
- $C_{A_i}$  is the concentration of trapped dopant  $A_i$ .
- $C_A^{ss}$  is the solid solubility of the dopant.
- $C_A^+$  is the active concentration of dopant  $A$ .

## 4: Diffusion

### Boundary Conditions

- $z$  is the charge state of the dopant.
- $E_{Rate}$  is the emission rate.

To set the model parameters, use:

```
pdbSet <interface material> <dopant> TrappingRate_<side> {<n>}
pdbSet <interface material> <dopant> EmissionRate_<side> {<n>}
pdbSet <interface material> CMax {<n>}
```

where `<side>` is one side of the interface and `<interface material>` is the interface material. For example, the side would be either Oxide or Silicon for an oxide–silicon interface.

Sentaurus Process allows the  $C_A^{T_{max}}$  parameter to be multiplied by user-defined factors as follows:

$$C_{A\text{Factor}}^{T_{max}} \times C_A^{T_{max}} \quad (668)$$

For example, in the case of an oxide–silicon interface, this is given by:

```
term name= CMaxFactor add Oxide /Silicon eqn= "exp(0.02)" store
```

To allow Sentaurus Process to use this term, specify a term with the name `CMaxFactor` for the interface material.

Similarly, you can modify  $T_{Rate}$  and  $E_{Rate}$  (the trapping and emission rates, respectively) using user-defined factors such as:

$$T_{Rate\text{-}Factor}} \times T_{Rate} \text{ and } E_{Rate\text{-}Factor}} \times E_{Rate} \quad (669)$$

The rate factors are specified as follows:

```
term name= <dopant>EmissionRateFactor_<side> add <InterfaceMaterial1> \
<InterfaceMaterial2> eqn= "<expr>" store
term name= <dopant>TrappingRateFactor_<side> add <InterfaceMaterial1> \
<InterfaceMaterial2> eqn= "<expr>" store
```

The factors are specified for an interface, for a particular dopant and specific to the side from which the interface is being approached. For example, given an oxide–silicon interface and an arsenic dopant, the `EmissionRateFactor` from the oxide side can be specified as:

```
term name= ArsenicEmissionRateFactor_Oxide add Oxide /Silicon \
eqn= "exp(2.0)" store
```

You also can use the individual trap density by switching off the `UseTotalInterfaceTrap` flag by:

```
pdbSet <interface material> <dopant> UseTotalInterfaceTrap 0
```

By default, the flag is switched off (0). If the flag is switched off, Eq. 667 becomes:

$$F_{a/b} = T_{Rate}^{a/b} ([C_A^{max}]^{a/b} - C_A) [C_A^+]^{a/b} \left( \frac{n}{n_i} \right)^z - E_{Rate}^{a/b} C_A \left( \frac{[C_A^{ss}]^{a/b} \cdot [C_A^{ss}]^{a/b}}{[C_A^{ss}]^{a/b} + [C_A^+]^{a/b}} \right) \quad (670)$$

where  $C_A^{max}$  is the maximum number of sites in the adjacent bulk region for this solution variable.

To change this parameter, use:

```
pdbSet <interface material> <dopant> CMax {<n>}
```

**NOTE** If the dopant diffusion model is set to `React` or `ChargedReact`,  $C_A^+$  will be the substitutional dopant.

Sentaurus Process allows the  $C_A^{max}$  parameter to be multiplied by user-defined factors as follows:

$$C_{AFactor}^{max} \times C_A^{max} \quad (671)$$

For example, in the case of specified boron at the oxide–silicon interface, this is given by:

```
term name= BoronCMaxFactor add Oxide /Silicon eqn= "exp(0.02)" store
```

To allow Sentaurus Process to use this term, specify a term with the name `<dopant>CMaxFactor` for the interface material.

Sentaurus Process also allows the parameter  $C_A^{ss}$  to be multiplied by a user-defined factor defined as `Side.SS.Factor`, for example:

```
pdbSetString Si B Side.SS.Factor "exp(3.636e-24*Pressure_Silicon/$kbT)"
```

## Surface Recombination Model: PairSegregation

If the Surface Recombination model is set to PairSegregation for the Pair or ChargedPair dopant diffusion model, the segregation fluxes are given by:

$$F_{a/b} = \left( \left[ \frac{C_I^0}{C_I^*} \right]^{a/b} f_I T_{Rate}^{a/b} + \left[ \frac{C_V^0}{C_V^*} \right]^{a/b} (1-f_I) T_{Rate}^{a/b} \right) \times \\ \left( \left[ [C_A^{Tmax}]^{a/b} - \sum_i C_{A_i} \right] [C_A^+]^{a/b} \left( \frac{n}{n_i} \right)^z - C_A [C_A^{ss}]^{a/b} \frac{E_{Rate}^{a/b}}{T_{Rate}^{a/b}} \right) \quad (672)$$

To use the total unpaired interstitial concentration, instead of the neutral one, use the command:

```
pdbSet <interface material> <dopant> UseUnpairedTotalInt <1 | 0 >
```

In this case,  $\left[ \frac{C_X^0}{C_X^*} \right]^{a/b}$  in Eq. 672 will be replaced with  $\left[ \frac{C_X}{C_X^*} \right]^{a/b}$ .

To enable explicit dependency of the emission flux from the interface to the material <side> on the active dopant concentration (similar to [Surface Recombination Model: Default on page 353](#)), use the command:

```
pdbSet <interface_material> <dopant> Emission.Active.Dependent_<side> <1 | 0 >
```

When this parameter is switched on for side a/b (by default, this parameter is switched off),

then  $[C_A^{ss}]^{a/b}$  in Eq. 672 and Eq. 673 is replaced by the expression  $\frac{[C_A^{ss}]^{a/b} \cdot [C_A]^{a/b}}{[C_A^{ss}]^{a/b} + [C_A^+]^{a/b}}$ .

If the surface recombination model is set to PairSegregation for the React or ChargedReact diffusion model, the segregation fluxes are given by:

$$F_{a/b} = \frac{f_I T_{Rate}^{a/b}}{[C_I^0]^{a/b}} \left( \left[ [C_A^{Tmax}]^{a/b} - \sum_i C_{A_i} \right] \frac{[C_{AI}]^{a/b} \left( \frac{n}{n_i} \right)^z}{\sum_z k_{AI}^{a/b} k_F^{a/b} \left( \frac{n}{n_i} \right)^{-z}} - C_A [C_A^{ss}]^{a/b} \frac{E_{Rate}^{a/b}}{T_{Rate}^{a/b}} [C_I^0]^{a/b} \right) \times \\ \frac{(1-f_I) T_{Rate}^{a/b}}{[C_V^0]^{a/b}} \left( \left[ [C_A^{Tmax}]^{a/b} - \sum_i C_{A_i} \right] \frac{[C_{AV}]^{a/b} \left( \frac{n}{n_i} \right)^z}{\sum_z k_{AV}^{a/b} k_V^{a/b} \left( \frac{n}{n_i} \right)^{-z}} - C_A [C_A^{ss}]^{a/b} \frac{E_{Rate}^{a/b}}{T_{Rate}^{a/b}} [C_V^0]^{a/b} \right) \quad (673)$$

where  $f_I$  is the interstitial fraction of dopant trapping in equilibrium and can be set using the command:

```
pdbSet <interface material> <dopant> Trap.Fi {<n>}
```

To use the total unpaired interstitial and vacancy concentration,  $f_I$  in Eq. 673 will be scaled with:

$$\frac{\sum_c k_{X^c} \left(\frac{n}{n_i}\right)^{-c}}{\sum_c k_{X^c}^s} \quad (674)$$

All other parameters have the usual meaning as explained above.

If the individual trap density is switched off,  $\left([C_A^{T_{max}}]^{a/b} - \sum_i C_{A_i}\right)$  will be replaced with  $([C_A^{max}]^{a/b} - C_A)$ .

$C_{AI}$  and  $C_{AV}$  are the concentrations of dopant-defect pairs.  $C_A$  is the concentration of the total unpaired dopant. If the surface recombination model is set to PairSegregation for the Constant, Fermi, or ChargedFermi diffusion model, the Default model will be used.

## ThreePhaseSegregation During SPER

During solid phase epitaxial regrowth (SPER), only solutions with nonzero `DAmorph` are solved, while the solutions in crystalline regions are frozen. Any diffusion model that takes into account pairs, such as `ChargedReact` or `Pair`, set by users has no effect in the material that has been amorphized.

In this case, a modified version of the `ThreePhaseSegregation` boundary condition is applied to interfaces with amorphous material. The equation for the segregation flux for the side that has been amorphized can be given by:

$$F_{a/b} = \text{AmorphState} \times \left( \text{AmT}_{\text{Rate}}^{a/b} \left( [C_A^{T_{max}}]^{a/b} - \sum_i C_{A_i} \right) [C_A]^{a/b} \left( \frac{n}{n_i} \right)^z - \text{AmE}_{\text{Rate}}^{a/b} C_A \right) \quad (675)$$

where:

- `AmorphState` is the fraction of the material in the amorphous state.
- `AmTRate` and `AmERate` are the trapping and emission rates for the amorphous phase of the material, respectively, and can be set by:

```
pdbSet Ox_Si As Amorphous.TrappingRate_Silicon <n>
pdbSet Ox_Si As Amorphous.EmissionRate_Silicon <n>
```

By default, `Amorphous.TrappingRate_<side>` takes the value of `TrappingRate_<side>`, and `Amorphous.EmissionRate_<side>` takes the value of `EmissionRate_<side>`.

---

## Trap

The Trap boundary condition is used to trap species at the interface. This boundary condition is a combination of the Segregation model (see [Segregation on page 348](#)) and the ThreePhaseSegregation model (see [ThreePhaseSegregation on page 352](#)).

The model is used mainly to trap nitrogen and fluorine during oxidation to reduce the oxidation rate (see [Trap-Dependent Oxidation on page 656](#)).

---

## TrapGen

The TrapGen boundary condition defines not only dopant trapping, but also dopant generation depending on the reaction velocity at a boundary.

---

## Continuous

For all of the same material interfaces (for example, Silicon\_Silicon), by default, continuous flux and solution boundary conditions apply:

$$C_1(x \rightarrow i) = C_2(i \leftarrow x) \quad (676)$$

$$D_1 \nabla C_1|_{n_1} = D_2 \nabla C_2|_{n_2} \quad (677)$$

where:

- Indices 1 and 2 indicate the two sides of the interface  $i$ .
- $n$  indicates the component of the dopant gradient normal to the interface.
- $D$  is the diffusivity, and  $C$  is the concentration of the solution variable.

If the boundary condition is not specified using the callback procedures for the solution variable at the interface, the continuous boundary condition can be set using the command:

```
pdbSetBoolean <mater> <dopant> Continuous 1
```

where  $<\text{mater}>$  is the interface material, and  $<\text{dopant}>$  is the solution variable name.

The following example sets the potential solution and its fluxes continuous at the polysilicon–silicon interface if Potential is solved on both sides of the interface:

```
pdbSetBoolean PolySilicon_Silicon Potential Continuous 1
```

---

## Dependency on Interface Crystal Orientation

Segregation of dopants at material interfaces (of crystalline or polycrystalline materials) can depend on the crystallographic orientation of the interfaces. For example, the surface density of atoms depends on the surface crystallographic orientation. It can be important to include orientation dependency in simulations of structures with multiple orientations present (or with nonflat interfaces), where interface orientation varies in space, for example, in FinFETs and trenches. Sentaurus Process supports orientation dependency of segregation parameters in the Segregation and ThreePhaseSegregation models.

Internally, Sentaurus Process computes the data fields Ori100, Ori110, and Ori111. These fields are the coordinates of a unit vector normal to the surface of a material relative to the basis (coordinate system) of the (nonorthogonal) unit vectors (100), (110), and (111) of the crystal. The surface normal vector is normalized such that  $Ori100 + Ori110 + Ori111 = 1.0$ . The following constant values are set for these data fields on the interface side of materials that are marked as amorphous in the PDB using <material> Amorphous 1:

```
Ori100=1.0, Ori110=0.0, Ori111=0.0
```

Linear interpolation of the segregation parameters is introduced between the three main symmetry axis orientations of the cubic crystal (100), (110), and (111). Therefore, this approach is good for cubic crystals due to their symmetry properties, but it is not sufficient for other crystal types. For example, for hexagonal crystals the three necessary basic directions are (100), (110), and (001) in the hexagonal crystal coordinate system.

**NOTE** Crystal types except for cubic crystal are not supported for orientation dependency segregation.

Segregation parameters depend on the crystal orientation at one (reference) side of the interface only, which is sufficient to simulate the case of amorphous–crystalline interfaces (for example, Oxide\_Silicon). This reference side is determined by the Segregation.Side.Aniso parameter, for example:

```
pdbSetString GaAs_Nitride Segregation.Side.Aniso GaAs
```

If the Segregation.Side.Aniso parameter is not present, or the material specified in it is amorphous (which is determined by the PDB parameter <material> Amorphous), no orientation dependency is applied to the segregation at this interface. In addition, no orientation dependency is applied to the segregation at the interfaces of the same materials.

To account for the orientation dependency, the segregation parameters described in [Segregation on page 348](#) and [ThreePhaseSegregation on page 352](#) are multiplied by the anisotropy prefactors of the orientation dependency. The prefactors  $k_{\text{aniso}}$  take the following general form:

$$k_{\text{aniso}} = k_{(100)}Ori100 + k_{(110)}Ori110 + k_{(111)}Ori111 \quad (678)$$

## 4: Diffusion

### Boundary Conditions

where  $Ori_{100}$ ,  $Ori_{110}$ , and  $Ori_{111}$  are the values of the corresponding fields at the reference side. The directional prefactors  $k_{\langle 100 \rangle}$ ,  $k_{\langle 110 \rangle}$ , and  $k_{\langle 111 \rangle}$  are defined by the corresponding PDB parameters of type double array:

```
pdbSet <interface_materials> <dopant> <segregation_parameter>.Fac.Aniso
```

or:

```
pdbSet <interface_materials> <dopant> <segregation_parameter>.Fac.Aniso_<side>
```

with the values  $\{100 \langle k_{100} \rangle 110 \langle k_{110} \rangle 111 \langle k_{111} \rangle\}$ , which are introduced on the same level as the corresponding segregation parameter ( $<\text{segregation\_parameter}>$ ). The following segregation parameters can be orientation dependent: Cmax, D, Segregation, Transfer, Trap.Fi, TrappingRate\_<side>, and EmissionRate\_<side>.

For example, orientation dependency for boron at the Oxide\_Silicon interface can be set by the following commands:

```
pdbSet Oxide_Silicon Boron Segregation.Side.Aniso Silicon
pdbSet Oxide_Silicon Boron CMax.Fac.Aniso      {100 1.0 110 1.0 111 1.0}
pdbSet Oxide_Silicon Boron D.Fac.Aniso        {100 1.0 110 1.0 111 1.0}
pdbSet Oxide_Silicon Boron Segregation.Fac.Aniso {100 1.0 110 1.0 111 1.0}
pdbSet Oxide_Silicon Boron Transfer.Fac.Aniso   {100 1.0 110 1.0 111 1.0}
pdbSet Oxide_Silicon Boron Trap.Fi.Fac.Aniso   {100 1.0 110 1.0 111 1.0}
pdbSet Oxide_Silicon Boron TrappingRate.Fac.Aniso_Oxide {100 1.0 110 1.0
111 1.0}
pdbSet Oxide_Silicon Boron TrappingRate.Fac.Aniso_Silicon {100 1.0 110 1.0
111 1.0}
pdbSet Oxide_Silicon Boron EmissionRate.Fac.Aniso_Oxide {100 1.0 110 1.0
111 1.0}
pdbSet Oxide_Silicon Boron EmissionRate.Fac.Aniso_Silicon {100 1.0 110 1.0
111 1.0}
```

If the directional segregation parameters:

```
pdbSet <interface_materials> <dopant> <segregation_parameter>.Fac.Aniso
```

or:

```
pdbSet <interface_materials> <dopant> <segregation_parameter>.Fac.Aniso_<side>
```

are not defined in the PDB, or all of the three prefactor values of the parameter are 0 or 1.0, the orientation dependency prefactors of these segregation parameters are not computed in Sentaurus Process and no orientation dependency for these parameters is used in the simulation. The default set of parameters results in the orientation dependency for segregation parameters being disabled.

**NOTE** The directional segregation parameters are subject to mole fraction-dependent parameter interpolation. Therefore, they must be defined for all the base interface materials involved to obtain the correct results when such interpolation is switched on.

---

## Periodic Boundary Condition

The periodic boundary condition can be applied when a device structure has a repetitive pattern:

```
 pdbSet Diffuse <Left | Right | Front | Back> Periodic <0 | 1>
```

The Front and Back definitions apply to 3D structures only.

---

## Boundary Conditions at Moving Interfaces

---

### Enhanced and Retarded Diffusion

During the growth of materials (for example, oxide and silicide), the reaction speed is calculated at the moving interfaces. The data field is called ReactionSpeed. The reaction speed can be used to simulate the enhanced dopant diffusion (for example, oxidation-enhanced diffusion (OED)) or the retarded dopant diffusion (for example, oxidation-retarded diffusion (ORD)) by allowing for the injection of interstitials and vacancies.

In [Eq. 643, p. 345](#), the injection rate is given as a function of the reaction speed ( $\|V_{ox}\| = \text{ReactionSpeed}$ ) and is used to simulate OED effects.

---

### Emulated Oxidation-Enhanced Diffusion

Moving boundaries especially in three dimensions has its own meshing challenges. It is very common to deposit a thick layer of oxide as a native layer to improve stability and performance in three dimensions, while allowing the boundary to move. In some cases, the required oxide thickness is deposited, and boundary movement is not allowed at all. In both cases, due to the reaction speed, OED effects will not be captured correctly.

To compensate for the thickness of the native layer, you can use the `emulated.oed` option of the `diffuse` command (see [diffuse on page 935](#)). If you specify this option, the reaction speed is calculated assuming a 1D structure where oxide is grown from an OED starting layer

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### Boundary Conditions at Moving Interfaces

thickness to that of the native layer thickness. The reaction speed is applied to the 1D, 2D, or 3D simulation structure during this process.

When the 1D oxidation thickness reaches the native layer thickness, the reaction speed is calculated using the simulation structure. The reaction speed from the 1D results is applied to all oxide–silicon interfaces. However, you can use the `emulated.oed.box` argument of the `diffuse` command to apply the reaction speed to a specific region. The OED starting layer thickness can be set using the command:

```
pdbSet Grid OED.Starting.Layer.Thickness <n>
```

If `OED.Starting.Layer.Thickness` is greater than `NativeLayerThickness`, emulation will not be switched on.

---

## Conserving Dose

The mesh of the simulated structure is modified during the growth of materials with each diffusion step. Some elements of the mesh will become bigger and some will shrink during this process. The change in the element size from one diffusion step to another will artificially change the dopant doses in the structure.

This artificial effect has two components. One is due to the change of element sizes and the other is due to the material consumption at the moving boundaries. The first effect is accounted for internally by applying an up-wind term to the solution equations. The second effect is accounted for using the Alagator scripting language. If the total dopant concentration on one side of the interface is different from the other side, the total concentration of the consumed material is used.

For example, if you assume that there are no dopant clusters and the `React` diffusion model for boron is selected on the silicon side and the `Constant` diffusion model is selected on the oxide side of an oxide–silicon interface, the total boron concentration would be `Boron+ BoronInt + BoronVac` on the silicon side and `Boron` on the oxide side. Since the consumed material is silicon during the oxidation, the dopant consumption due to growth is passed using the command:

```
pdbSetString Oxide_Silicon Boron Consumed_Silicon \
    "Boron_Silicon+BoronInt_Silicon+BoronVac_Silicon"
```

This is performed automatically. If the `React` diffusion model for boron was also selected on the oxide side, the total dopant concentration on the oxide side would be `Boron+ BoronInt + BoronVac`, and the following command would be used:

```
pdbSetString Oxide_Silicon Boron Consumed_Silicon "Boron_Silicon"
```

## Common Dopant and Defect Dataset Names

Sentaurus Process does not solve the diffusion equations for the total dopant or defect concentrations, but solves the equations for the total unpaired dopant and defect concentrations. Sentaurus Process monitors the total dopant and defect concentration through various terms. Depending on the diffusion models selected, Sentaurus Process will update these terms. For example, the commands:

```
pdbSet Silicon Dopant DiffModel React
pdbSet Silicon B ActiveModel None
```

will set the dopant diffusion model in silicon to React and the active model to None for boron in silicon. Assuming that there is only boron in the structure, various terms and data fields will be created after the diffusion. The most important ones are Boron, BActive, BTotal, BoronInt, BoronVac, Int, ITTotal, Interstitial, Vac, VacTotal, and Vacancy. Boron, BoronInt, BoronVac, Int, and Vac are the solution names.

**Table 43 Terms and data fields created after diffusion with React diffusion model and None activation model for boron**

Term or data field	Description
BActive	Active boron concentration. (Since the active model is none, it will be equal to Boron).
Boron	Total unpaired boron concentration (for example, no clusters, no boron–defect pairs).
BoronInt	Concentration of boron–interstitial pairs.
BoronVac	Concentration of boron–vacancy pairs.
BTotal	Boron + BoronInt + BoronVac = Total boron concentration.
Int	Total unpaired interstitial concentration.
Interstitial	Total interstitial concentration used to initialize Int. (In this example, it will be Int.)
ITTotal	Int + BoronInt = Total interstitial concentration.
Vac	Total unpaired vacancy concentration.
Vacancy	Total vacancy concentration used to initialize Vac. (In this example, it will be Vac.)
VTotal	Vac + BoronVac = Total vacancy concentration.

If the following cluster models for both interstitial and boron are switched on, some of the previous fields will be updated:

```
pdbSet Si Dopant DiffModel React
pdbSet Si B ActiveModel Transient
pdbSet Si I ClusterModel 1Moment
```

## 4: Diffusion

### Common Dopant and Defect Dataset Names

Two additional solution variables will be solved:

- ICluster is the clustered interstitials used with the 1Moment model (see [Defect Cluster Model: 1Moment on page 323](#)).
- B4 is the clustered boron used with the Transient model (see [Dopant Active Model: Transient on page 283](#)).

The changed fields will be:

BTotal              Boron + 4\*B4 + BoronInt + BoronVac = Total boron concentration.

ITotal              Int + BoronInt + ICluster = Total interstitial concentration.

If the diffusion and cluster models are changed as follows:

```
pdbSet Si Dopant DiffModel ChargedPair  
pdbSet Si B ActiveModel Transient  
pdbSet Si I ClusterModel Equilibrium
```

Sentaurus Process uses the ChargedPair diffusion model (see [ChargedPair Diffusion Model on page 185](#)), and the Transient active model (see [Dopant Active Model: Transient on page 283](#)) for boron, and the Equilibrium cluster model (see [Defect Cluster Model: Equilibrium on page 307](#)) for interstitials.

In this case, Boron, B4, Int, and Vac will be the solution names. BoronInt and BoronVac will not be solved, but there will be BoronInt and BoronVac terms to calculate boron–interstitial and boron–vacancy concentrations. In this case, total unpaired Boron also will include BoronInt and BoronVac since they are not solved. [Table 44](#) lists the important fields.

Table 44 Terms and data fields created after diffusion with React diffusion model and Transient activation model for boron, and 1Moment cluster model

Data field	Description
BActive	Boron – BoronInt – BoronVac = Active boron concentration.
Boron	Total unpaired boron concentration.
BoronInt	Concentration of boron–interstitial pairs calculated using <a href="#">Eq. 124, p. 178</a> .
BoronVac	Concentration of boron–vacancy pairs calculated using <a href="#">Eq. 124</a> .
BTotal	Boron + 4*B4 = Total boron concentration.
ICluster	Equilibrium interstitial concentration calculated using <a href="#">Eq. 493, p. 307</a> .
Int	Total unpaired interstitial concentration.
Interstitial	Int + 4*ICluster + BoronInt = Total interstitial concentration used to initialize Int.

Table 44 Terms and data fields created after diffusion with React diffusion model and Transient activation model for boron, and 1Moment cluster model

Data field	Description
ITotal	Int + 4*ICluster + BoronInt = Total interstitial concentration.
Vac	Total unpaired vacancy concentration.
Vacancy	Vac + BoronVac = Total vacancy concentration used to initialize Vac.
VTotal	Vac + BoronVac = Total vacancy concentration.

**NOTE** If the dopant, defect, or cluster fields are modified by other process steps (for example, implantation or deposition), terms that define active dopant concentration and total dopant concentration may not be current. They are updated in the next diffusion step.

Table 45 Variable names used in diffusion and reaction solvers

Name	Comment	Solution (S), Term (T), Data field (F)
Antimony	Total unpaired antimony concentration	S, F
AntimonyGbc	Antimony grain boundary concentration	S, F
AntimonyInit	Antimony–interstitial pair concentration	T or (S, F) (depends on the model)
AntimonyVac	Antimony–vacancy pair concentration	T or (S, F) (depends on the model)
Arsenic	Total unpaired arsenic concentration	S, F
ArsenicGbc	Arsenic grain boundary concentration	S, F
ArsenicInt	Arsenic–interstitial pair concentration	T or (S, F) (depends on the model)
ArsenicVac	Arsenic–vacancy pair concentration	T or (S, F) (depends on the model)
As3	Three-arsenic cluster concentration (default size is three, user-configurable)	S, F
As4Vac	Four-arsenic and a vacancy cluster concentration	S, F
AsActive	Arsenic active concentration	T
AsTotal	Total arsenic concentration	T (for example, Arsenic+4*As4Vac)
B2	Two-boron cluster concentration	S, F
B2I	Two-boron and interstitial cluster concentration	S, F
B2I2	Two-boron and two-interstitial cluster concentration	S, F

#### 4: Diffusion

##### Common Dopant and Defect Dataset Names

Table 45 Variable names used in diffusion and reaction solvers

Name	Comment	Solution (S), Term (T), Data field (F)
B2I3	Two-boron and three-interstitial cluster concentration	S, F
B3	Three-boron cluster concentration	S, F
B3I	Three-boron and interstitial cluster concentration	S, F
B3I2	Three-boron and two-interstitial cluster concentration	S, F
B3I3	Three-boron and three-interstitial cluster concentration	S, F
B3I4	Three-boron and four-interstitial cluster concentration	S, F
B4	Four-boron cluster concentration (default size is four, user-configurable)	S, F
BActive	Boron active concentration	T
BI2	Boron and two-interstitial cluster concentration	S, F
Boron	Total unpaired boron concentration	S, F
BoronGbc	Boron grain boundary concentration	S, F
BoronInt	Boron–interstitial pair concentration	T or (S, F) (depends on the model)
BoronVac	Boron–vacancy pair concentration	T or (S, F) (depends on the model)
BTotal	Total boron concentration	T (for example, Boron+2*B2I)
C2	Two-carbon cluster concentration	S, F
C2I	Two-carbon and interstitial cluster concentration	S, F
C3I1	Concentration of interstitials trapped in {311} defects	S, F
C3I	Three-carbon and interstitial cluster concentration	S, F
C3I2	Three-carbon and two-interstitial cluster concentration	S, F
C4I2	Four-carbon and two-interstitial cluster concentration	S, F
C4I3	Four-carbon and three-interstitial cluster concentration	S, F
C5I3	Five-carbon and three-interstitial cluster concentration	S, F

Table 45 Variable names used in diffusion and reaction solvers

Name	Comment	Solution (S), Term (T), Data field (F)
C5I4	Five-carbon and four-interstitial cluster concentration	S, F
C6I5	Six-carbon and five-interstitial cluster concentration	S, F
C6I6	Six-carbon and six-interstitial cluster concentration	S, F
Carbon	Total unpaired carbon concentration	S, F
CarbonInt	Carbon–interstitial pair concentration	S, F
CLoop	Concentration of interstitials trapped in dislocation loops	T or (S, F) (depends on the model)
CTotal	Total carbon concentration	T
D311	Density of {311} defects	S, F
DLoop	Density of dislocation loops	T or (S, F) (depends on the model)
EqInt	Equilibrium interstitial concentration	T
EqVac	Equilibrium vacancy concentration	T
F3V	Three-fluorine and vacancy cluster concentration	S, F
Fluorine	Total unpaired fluorine concentration	S, F
FluorineTotal	Total fluorine concentration	T
GeB	Germanium–boron pair concentration	S, F
Germanium	Total unpaired germanium concentration	S, F
GermaniumTotal	Total germanium concentration	T
GSize	Grain size	S
H2O	Wet oxidant concentration	S, F
I2	Two-interstitial cluster concentration	S, F
ICluster	Interstitial cluster concentration	T or (S, F) (depends on the model)
In3	Three-indium cluster concentration (default size is three, user-configurable)	S, F
InActive	Indium active concentration	T
Indium	Total unpaired indium concentration	S, F
IndiumGbc	Indium grain boundary concentration	S, F
IndiumInt	Indium–interstitial pair concentration	T or (S, F) (depends on the model)

#### 4: Diffusion

##### Common Dopant and Defect Dataset Names

Table 45 Variable names used in diffusion and reaction solvers

Name	Comment	Solution (S), Term (T), Data field (F)
IndiumVac	Indium–vacancy pair concentration	T or (S, F) (depends on the model)
Int	Total unpaired interstitial concentration	S, F
Interstitial	Total interstitial concentration excluding cluster solutions, used to initialize Int	F
IntNeutral	Neutral interstitial concentration ( $I_0$ )	T
InTotal	Total indium concentration	T
IntTotal	Total interstitial concentration	T
O2	Dry oxidant concentration	S, F
P3	Three-phosphorus cluster concentration (default size is three, user-configurable)	S, F
PActive	Phosphorus active concentration	T
Phosphorus	Total unpaired phosphorus concentration	S, F
PhosphorusGbc	Phosphorus grain boundary concentration	S, F
PhosphorusInt	Phosphorus–interstitial pair concentration	T or (S, F) (depends on the model)
PhosphorusVac	Phosphorus–vacancy pair concentration	T or (S, F) (depends on the model)
Potential	Electrostatic potential	T or (S, F) (depends on the model)
PTotal	Total phosphorus concentration	T
Sb3	Three-antimony cluster concentration (default size is three, user-configurable)	S, F
SbActive	Antimony active concentration	T
SbTotal	Total antimony concentration	T (for example, Antimony+AntimonyVac)
Smic	Concentration of submicroscopic interstitial clusters (default size 4)	S, F
SmicS	Concentration of smaller submicroscopic interstitial clusters (default size 2)	S, F
V2	Two-vacancy cluster concentration	S, F
Vac	Total unpaired vacancy concentration	S, F
Vacancy	Total vacancy concentration excluding cluster solutions, used to initialize Vac	F
VacNeutral	Neutral vacancy concentration ( $V_0$ )	T
VacTotal	Total vacancy concentration	T

---

## References

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# Atomistic Kinetic Monte Carlo Diffusion

---

*This chapter describes the atomistic simulation approach to diffusion and activation processes in Sentaurus Process, as well as alternatives for faceted solid phase epitaxial regrowth.*

All diffusion models described in [Chapter 4 on page 167](#) are based on the conventional (continuum) simulation approach. The atomistic approach described here is based partially on the kinetic Monte Carlo (KMC) diffusion simulator DADOS [\[1\]](#)[\[2\]](#)[\[3\]](#) and is available with the optional Sentaurus Process Kinetic Monte Carlo license.

---

## Overview

The continuum approach to modeling dopant diffusion in process simulation tools is used to solve a system of partial differential equations (PDEs) that describe transport of the dopants and conservation of the dose. This approach has been useful in designing semiconductor devices in the past, but trends in the manufacturing process of sub-100-nm devices may make it difficult to maintain a high predictability in future devices.

The shrinking thermal budget significantly reduces diffusion and, therefore, reduces the need to accurately model diffusion. On the other hand, dopant activation phenomena, including the formation of a variety of dopant–defect pairs and extended defects of different configurations, often do not reach thermodynamic equilibrium and necessitate transient rather than equilibrium simulation. In the continuum diffusion model, this requires the use of one equation per each dopant–defect configuration, which leads to a multitude of equations to be solved.

The trend of reducing device sizes results in a small number of impurity atoms (as small as tens or hundreds) that determine the threshold voltage of a transistor. It is likely that a limit soon will be reached where small discretized distribution can no longer be accurately modeled with a continuum description.

A Monte Carlo (MC)–based diffusion simulation provides a valuable alternative to the continuum approach. Computational resources required for MC diffusion simulation are decreasing with device dimension because they are proportional to the number of dopants and defects in the device. On the other hand, resources for continuum simulations increase as modeling of ever more complex nonequilibrium phenomena are required. This trend has

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Operating Modes

already gone a long way towards making the KMC diffusion method competitive with the most detailed continuum diffusion methods today in terms of the required computational resources.

Unlike the continuum approach, the large number of different dopant–defect configurations does not present a problem for the MC approach, which simply needs to introduce the probabilities for the additional reactions. These probabilities are calculated based on the binding energies that can be plugged in directly from experiments, molecular dynamics, or *ab initio* calculations.

In addition, atomistic implantation and diffusion models provide a way of determining statistical variations for a specific process flow–device geometry combination.

---

## Kinetic Monte Carlo Method

Sentaurus Process Kinetic Monte Carlo (Sentaurus Process KMC) considers only defects and impurities, and ignores the lattice (except for some solid phase epitaxial regrowth (SPER) and epitaxial deposition models). This drastically reduces memory requirements compared to molecular dynamics or lattice KMC techniques and allows you to investigate simulation domains that are large enough to contain deep-submicron devices. As Sentaurus Process KMC tracks the diffusion and interaction of defects, the fastest process is the jumping of a point defect with a period of approximately  $10^{-9}$  s. When there are no mobile point defects in the structure, the time step is increased automatically to an emission of mobile particles from the surface or from an extended defect, which has a period of approximately  $10^{-3}$  s.

Therefore, typically, Sentaurus Process KMC would begin with time steps of approximately  $10^{-9}$  s. As the point defects are trapped by the clusters and extended defects, Sentaurus Process KMC switches automatically to larger time steps of the order of  $10^{-3}$  s, which are large enough to model typical process steps.

---

## Operating Modes

Sentaurus Process KMC can operate in different modes as follows:

- The *atomistic* mode handles data atomistically throughout the simulation and is expected to be the most accurate method.
- The *nonatomistic* mode allows Sentaurus Process KMC to be used for only part of a simulation. Sentaurus Process KMC transfers data back and forth to the continuum solver to allow you to take advantage of the efficiency of the continuum solver for steps closer to equilibrium and to allow Sentaurus Process KMC to handle one or more steps that are far from equilibrium (such as rapid thermal annealing) to take advantage of its accuracy.

## Atomistic Mode

When Sentaurus Process KMC is in atomistic mode, the data fields are handled completely atomistically. To select the atomistic mode at the very beginning of the simulation, use:

```
SetAtomistic
```

The `SetAtomistic` command sets the parameter `AtomisticData` to `true`, allowing the Sentaurus Process commands listed in [Table 46](#) to work in atomistic mode whenever possible, and to properly synchronize Sentaurus Process KMC when the structure changes. The `SetAtomistic` command also sets the diffusion method as Sentaurus Process KMC, and the implantation mode as MC implantation. Finally, it calls `PDE2KMC` to atomize the available continuum fields into atomistic ones. To exit the atomistic mode, use:

```
UnsetAtomistic
```

The `UnsetAtomistic` command calls the procedure `KMC2PDE` to translate the atomistic quantities to fields and exits the atomistic mode.

When `AtomisticData` is `true`, Sentaurus Process KMC does not populate continuum data fields with its own results, unless instructed to do so (using `kmc deatomize`).

## Restrictions

The following restrictions apply when using the atomistic mode:

- Do not use the command `transform stretch`.
- The `load` command only accepts the arguments `tdr` and `replace`.

The other commands work as expected, although those listed in [Table 46](#) have been especially adapted to operate in the atomistic mode.

**Table 46** Commands adapted to work in atomistic mode

Command	Description of adaptation
<code>deposit</code>	Synchronizes the Sentaurus Process KMC structure after deposition.
<code>diffuse</code>	If the parameter <code>kmc</code> is specified or <code>Diffuse KMC 1</code> is set in the parameter database, <code>diffuse</code> calls Sentaurus Process KMC. If <code>AtomisticData 1</code> is not set, a new KMC object is created, and it will be removed at the end of the diffusion step. Oxidation, nitridation, epitaxial deposition, and so on are accepted.
<code>etch</code>	Synchronizes the Sentaurus Process KMC structure removing the etched material and its contained particles, and setting the material to gas.
<code>implant</code>	Uses MC implantation and sends the cascades directly to Sentaurus Process KMC. Dynamic annealing also is simulated during the implantation using Sentaurus Process KMC.

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Operating Modes

Table 46 Commands adapted to work in atomistic mode

Command	Description of adaptation
init	If a background concentration is specified, it is atomized and passed as particles to Sentaurus Process KMC.
line	Adds a new line to the Sentaurus Process KMC internal mesh, when possible.
load	Loads a Sentaurus Process KMC distribution from a TDR file and replaces the current one.
math	Accepts numThreadsKMC.
photo	Creates photoresist mask and synchronizes the new Sentaurus Process KMC structure.
profile	Loads and atomizes a profile.
region	When <code>region</code> changes the material, Sentaurus Process KMC is synchronized.
select	(Only when <code>select</code> creates a new field or modifies an existing one). If this field is known by Sentaurus Process KMC, the Sentaurus Process KMC concentration of particles is synchronized with the value of the field, removing or creating extra particles.
strip	Sentaurus Process KMC is synchronized with the new material. If there are particles in the stripped materials, they are removed.
struct	Automatically deatomizes some Sentaurus Process KMC data fields to make them accessible when saving to a file. It also saves Sentaurus Process KMC restart information.
transform	The Sentaurus Process KMC structure is updated after the transformation. Particles are removed or modified depending on the particular materials being created or removed. The option <code>stretch</code> is not allowed.

## Implantation

Sentaurus Process KMC requires the damage morphology (coordinates of each point defect) for its damage accumulation model; this information is not available in analytic implantations. In atomistic mode, the `implant` command automatically uses the Sentaurus MC engine as well as the `cascades` option for storing full cascades. The implantation time also is needed because, while implanting, Sentaurus Process KMC automatically performs diffusion at the specified temperature (default is ambient). Typically, the temperature and time during the implantation affect only slightly the distribution of dopants, but they may affect damage accumulation, amorphization, and subsequent recrystallization and impurity cluster formation. The implantation time is returned by the function `DoseRate` defined in the `Implant.tcl` file. This time is computed by default using a fixed dose rate equal to  $1 \times 10^{12} / \text{cm}^2 \text{s}$ . If a dose rate is specified in an `implant` command by the `dose.rate` argument, it is used to compute the implantation time for this particular implantation instead.

For each implantation dose and surface size, the number of implanted ions is computed. For example,  $1 \times 10^{14} \text{ cm}^{-2}$  boron dose in a simulation cell with a surface of  $40 \times 40 \text{ nm}^2$  and 250-nm depth implantations  $40 \times 10^{-7} \times 40 \times 10^{-7} \times 10^{14} = 1600$  boron cascades (being a cascade, one ion and all its generated damage). The information is passed to Sentaurus

Process KMC for annealing. These diffusion steps occur internally and are not user specified, but the total ‘diffused’ time can be controlled by the function `DoseRate`. Afterwards, the implantation report issued by Sentaurus Process KMC names the backscattered particles as *outside* particles.

Molecular implantations are allowed. To perform a molecular implantation, specify the name of the molecule as the implantation species (see [Chapter 3 on page 53](#)). The components of implanted molecules are introduced as isolated species in Sentaurus Process KMC; in other words, an implanted BF2 molecule will split into 2F and 1B inside Sentaurus Process KMC.

## Diffusion

For the first diffusion step after implantation, using a small temperature ramp-up is recommended. The time for this ramp-up should be chosen as realistically as possible. At the end of an implantation, the simulation cell contains the implanted ions plus a large amount of damage (point defects). During the ramp-up, this damage recombines and forms different cluster types. The use of a realistic ramp-up produces more accurate results.

You can set the pdb parameters `automaticRampUp` and `automaticRampDown` to `true` to automatically perform ramps whenever the requested diffusion temperature differs from the current one. These ramps are performed with a ramp rate specified by `rampUpRate` and `rampDownRate` in C/s:

```
sprocess> pdbGet KMC rampUpRate
100
sprocess> pdbGet KMC automaticRampUp
0
```

Sentaurus Process KMC performs different annealings at different temperatures during the ramp-up. The objective is to perform a few large anneals at low temperature and short ones at high temperatures. This maintains a high accuracy without spending too much time at low temperatures (changes in the temperature have a performance penalty).

The way these ramp-ups are performed can be configured using the following parameters of the parameter database:

```
sprocess> pdbGet KMC dTBase
2.0
sprocess> pdbGet KMC nInit
1
sprocess> pdbGet KMC dTLimit
20.0
```

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Operating Modes

The temperature steps for the highest temperature (the end of the ramp-up or the beginning of the ramp-down) are computed as:

$$(\Delta T_{base})^{n_{init} + n} \quad (679)$$

where  $\Delta T_{base}$  is dTBase and  $n_{init}$  is nInit.

For example, using the above parameters, in a ramp-down from 600°C to 500°C, the first annealing is performed at  $600^{\circ}\text{C} - 2^{1+0} = 598^{\circ}\text{C}$ , the second one is performed at  $598^{\circ}\text{C} - 2^{1+1} = 594^{\circ}\text{C}$ , and so on. When  $(\Delta T_{base})^{n_{init} + n}$  is greater than dTLimit, the value dTLimit is taken.

**NOTE** These parameters are used only for temperature ramps induced by automaticRampUp or automaticRampDown. For temperature ramps specified with the temp\_ramp command, the parameters to control the ramp are specified in the temp\_ramp or diffuse command.

Oxidation and silicidation options are allowed in Sentaurus Process KMC. See [Oxidation-Enhanced Diffusion \(OED\) Model on page 511](#), [Oxidation on page 517](#), and [Silicidation on page 518](#).

---

## Nonatomistic Mode

Sentaurus Process KMC also can be used only for one diffusion step, synchronizing the status of the simulation before and after the diffusion step. This is performed with the kmc argument in the diffuse command as follows:

```
diffuse kmc temperature=<n> time=<n>
```

When Sentaurus Process KMC runs with AtomisticData set to false, a new Sentaurus Process KMC simulation is launched at the beginning of the diffuse command:

- First, it receives the information (atomized from the data fields).
- Second, the diffusion is completed and, at the end of this command, Sentaurus Process KMC transfers the information to Sentaurus Process as data fields.
- Third, the Sentaurus Process KMC information is removed from memory.

This is similar to the following commands:

```
SetAtomistic  
diffuse temperature=<n> time=<n>  
UnsetAtomistic
```

---

## Translating Atomistic and Nonatomistic Information

Transformations of information back and forth from concentrations to particles are performed by the Tcl procedures `PDE2KMC` and `KMC2PDE`. These transformations may degrade the accuracy of the obtained results. By default, the transformation to continuum data is mapped to the `ChargedReact` (five-stream) model.

If you need a customized transformation, you can rewrite the procedures `PDE2KMCUser` and `KMC2PDEUser` with your own map. `PDE2KMCUser` (or `KMC2PDEUser`) returns a string mapping the array of transformation from continuum to atomistic (or atomistic to continuum). `KMC2PDEUser` cannot modify already existing fields, but it can add new ones. These maps contain three columns: the name of the original field, the name of the translated field, and the factor to be applied during the translation. For example, the following will transfer a new helium field into Sentaurus Process KMC:

```
fproc PDE2KMCUser {} {  
    return "Helium He 1 \  
           HeInt Hei 1 \  
           HeVac HeV 1"  
}
```

`PDE2KMC` uses the Parameter Database (PDB) parameter `KMC Si Damage TrimField` to trim the PDE fields that exceed this maximum value. It is useful to trim the concentration of Is and Vs in amorphized regions to more realistic values, avoiding the wasteful creation of excessive point defects. A value being at least 20% higher than the Sentaurus Process KMC amorphization threshold is suggested to properly amorphize the material.

In addition to the standard translations, there are special built-in translations for total concentrations such as `BTOTAL` (`BoronConcentration`) and `ASTOTAL` (`ArsenicConcentration`), and for the field `NetActive` (`DopingConcentration`). The computation of the total concentration is performed for dopants and germanium, and takes into account all species. For example, Bi contributes one boron atom to `BTOTAL`, and `B2I3` contributes two boron atoms. The field `NetActive` is computed by summing all charged particles including substitutional dopants, charged dopant-defect pairs, charged clusters, and so on. The `NetActive` field is only computed in materials in which the Boolean PDB parameter `KMC <material> Semiconductor` is true.

For further customization, you can overload the Tcl procedures with your own. For more information on how to create and manipulate continuum and atomistic data, see [kmc on page 1037](#) and [select on page 1168](#).

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Operating Modes

**NOTE** KMC2PDE and PDE2KMC may consume a large amount of CPU time in large simulations. To improve efficiency, KMC2PDE keeps track of a previous translation and does not perform a new one if the previous one is still valid.

## Sano Method

The Sano method converts particles to continuum profiles inside Sentaurus Process. The conversion is performed using the same module as the one available in Sentaurus Mesh.

For details, see [Sentaurus™ Mesh User Guide, Defining Particle Profiles on page 17](#) and [Sentaurus™ Mesh User Guide, Appendix B on page 123](#).

To apply the Sano method to all dopants and the computed quantity `NetActive`, select the `sano` option of the `UnsetAtomistic` command. However, to take full advantage of having the Sano method inside Sentaurus Process:

1. Generate a mesh tailored for device simulation, including the use of adaptive refinement based on `NetActive`.
2. Add contacts using the `contact` command.
3. Use `tdr=<c> !Gas` in the `struct` command, which creates, by default, a mesh with contacts present and appropriate for device simulation.

As an example:

```
# Place mesh settings before UnsetAtomistic command in 3D, because a new mesh
# will be created during UnsetAtomistic using the current refinement settings

pdbSet Grid Adaptive 1
refinebox adaptive refine.fields= {BActive AsActive NetActive} \
    rel.error= {BActive= 1.1 AsActive= 1.1 NetActive= 1e30} \
    max.asinhdiff= {NetActive= 5} target.length= 1e5 refine.min.edge= 0.5<nm>
UnsetAtomistic sano

contact name= c1 box xlo= 0.0 ylo= 0.0025 xhi= 0.04 yhi= 0.0125 silicon \
    adjacent.material= oxide
contact name= c2 box xlo= 0.025 ylo= -0.01 xhi= 0.075 yhi= 0.01 silicon
struct tdr= n10 !Gas
```

The following parameter controls the accuracy of the Sano smoothing computation:

```
pdbSet KMC SanoMethod <species> ScreeningFactor <n>
```

The screening factor sets the inverse of the screening length of the Sano method. The smaller the screening factor, the smoother the profile and the longer the computation time.

For more options of the `UnsetAtomistic` command, see [UnsetAtomistic on page 1252](#). In addition, smoothing and remeshing based on Sano fields can be called directly using the `grid` command (see [grid on page 974](#)).

---

## Simulation Domain

All Sentaurus Process KMC simulations are performed internally in a 3D domain. If the Sentaurus Process structure is 1D or 2D, the missing lateral dimensions are created automatically to form a 3D simulation domain for Sentaurus Process KMC. For a 2D structure, the extension in the z-direction is taken from `MinZum` and `MaxZum`. For a 1D structure, the default extension is `MinYum` to `MaxYum` and `MinZum` to `MaxZum`.

To change the default values, use:

```
pdbSet KMC MinYum <n>
pdbSet KMC MaxYum <n>
```

The Sentaurus Process KMC simulation domain is the same as the Sentaurus Process simulation domain, including the top of the simulation, and it cannot be changed. For Y and Z, the values `MinYum`, `MinZum` and `MaxYum`, `MaxZum` are used only when they are not set up in the command file (because the dimensionality of the simulation is smaller).

Consequently, the Sentaurus Process KMC dimensions fit Sentaurus Process dimensions. The size of the Sentaurus Process KMC simulation domain is reported in the output, for example:

```
KMC domain (-0.1, 0, 0) to (0.02, 0.02, 0.025) um Sentaurus domain (-0.1, 0, 0)
to (0.02, 0.02, 0) um.
```

---

## Recommended Domain Size

For 3D simulations of deep-submicron transistors with twofold symmetry, you should make the size of the simulation domain one-quarter of the transistor size. The Sentaurus Process KMC domain is automatically the same.

For a 1D simulation (that can be compared to SIMS data), Sentaurus Process KMC uses as small as possible lateral domain sizes to save CPU time. However, simulation domains with lateral sizes smaller than 20 nm may be too small to represent extended defects. If you are interested in a 1D profile with less statistical noise, you should increase the lateral size.

**NOTE** The minimum recommended size for accurate implantation cascades and damage accumulation is  $40 \times 40 \text{ nm}^2$ .

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Internal Grid

The lateral domain area is multiplied by the implantation dose to obtain the number of ions implanted. For high impurity concentration levels, you may obtain enough particles in a relatively small simulation domain. For example, the implantation dose of  $10^{15} \text{ cm}^{-2}$  creates 16000 ions for the  $40 \times 40 \text{ nm}^2$  lateral domain side. This might be sufficient to obtain low statistical noise, while any further increase in the  $40 \times 40 \text{ nm}^2$  lateral domain size only slows the simulation.

To obtain good statistics for lower concentrations or lower doses, you must increase the lateral size of the simulation domain. For example, an implantation dose of  $10^{12} \text{ cm}^{-2}$  creates only 16 ions for the  $40 \times 40 \text{ nm}^2$  lateral domain.

One way to reduce the statistical noise without increasing the waiting time is to use multithreading, available for 1D and 2D simulations (see [Parallelism on page 385](#)).

**NOTE** When using Sentaurus Process KMC, try to use the smallest (but still realistic) domain possible. If the simulation is too noisy or not representative, increase the lateral size. CPU time typically is proportional to the surface area. If a simulation with a  $20 \times 20 \text{ nm}^2$  surface takes 5 minutes to finish, you can expect a  $40 \times 40 \text{ nm}^2$  simulation to take four times longer.

---

## Internal Grid

Sentaurus Process KMC uses an internal grid to:

- Store the geometry and material assignments of the structure being simulated.
- Accelerate the search for possible interaction partners for each defect in the simulation.
- Compute the electronic properties.
- Be the minimum volume of amorphized silicon.
- Be the basis for computing the concentrations written in the TDR file (using the `kmc extract tdrWrite` command).

The Sentaurus Process KMC grid is a tensor-product grid. This grid is different and isolated from the regular Sentaurus Process grid. The minimum size for each rectangular grid box is set to  $0.4 \times 0.4 \times 0.4 \text{ nm}^3$ , and a minimum value  $< 0.4 \text{ nm}$  in any axis will not be accepted. There is no maximum size. The grid is built using Sentaurus Mesh and can be adjusted using the PDB parameters listed in [Table 47 on page 383](#).

Table 47 PDB parameters for modifying grid

Parameter	Default value	Description
Always3DMeshing	false	Use Sentaurus Mesh to extrude 2D into 3D. By default, it uses an internal algorithm.
NonUniformTensor		Use a nonuniform tensor grid (true) or use the old uniform tensor method (false) and the obsolete parameters BitsBoxes and MinXum. <b>NOTE</b> Using the old uniform tensor method is strongly discouraged.
XGrading	1.05	Grading in the x-direction.
YMaxCell	2.5 nm	Maximum cell size in y-direction [ $\mu\text{m}$ ].
YMinCell	1.5 nm	Minimum cell size in y-direction [ $\mu\text{m}$ ].
ZMaxCell	2.5 nm	Maximum cell size in z-direction [ $\mu\text{m}$ ].
ZMinCell	1.5 nm	Minimum cell size in z-direction [ $\mu\text{m}$ ].

**NOTE** The smallest minimum grid size allowed is  $4.0 \times 10^{-4} \mu\text{m}$ , which corresponds to the hopping distance. To achieve this minimum mesh spacing, in addition to setting YMinCell, or ZMinCell, or both to 4.0e-4, specify spacing=4<nm> in the line command along with the following PDB setting to control mesh lines precisely:

```
pdbSet Grid KMC UseLines 1
```

**NOTE** If the minimum grid size (YMinCell or ZMinCell) is set to less than 0.8 nm, the long hopping models are disabled.

There are no XMinCell and XMaxCell for the x-direction. The maximum size for x is fixed to 100 nm, but it is further controlled with refinements, as explained here. The final mesh is similar to the one obtained by Sentaurus Mesh using the following script:

```
tensor {
    mesh {
        mincellsize = 8e-4
        maxcellsize direction "x" 1e-1
        maxcellsize direction "y" $YMaxCell
        mincellsize direction "y" $YMinCell
        maxcellsize direction "z" $ZMaxCell
        mincellsize direction "z" $ZMinCell
        minbndcellsize = 8e-4
        maxbndcellsize = 1e-3
        grading = {$XGrading $XGrading}
    }
}
```

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Randomization

where \$Name is the value of the parameter. The default parameters are set to try to minimize the Manhattan geometry at the interfaces, while maximizing the performance of the simulation. All of these parameters can be set using `pdbSet KMC`, for example:

```
pdbSet KMC ZMaxCell 3e-3
```

Further customization can be added in the form of refinements. To refine the KMC internal grid, use the `refinebox kmc` command. By default, Sentaurus Process KMC applies one refinement when using `SetAtomistic`. This refinement is defined as:

```
refinebox kmc min= {0 0} max= {0.1 2} xrefine= {0.0012 0.0015 0.0015}
```

This default refinement can be changed by overwriting the `kmcDefaultRefinement` procedure with a user-defined refinement. For example, to remove the default refinement only, use:

```
fproc kmcDefaultRefinement { } {
   LogFile "Removing the default refinement (by not defining it)..."
```

Finally, the lines and spacing specified with the `line` command also will be included in the simulation if possible.

For more information on the internal grid and how it affects the simulation, see [Materials and Space on page 391](#).

---

## Randomization

You can investigate statistical variations of a process flow by selecting a different seed for the random number generator used by Sentaurus Process KMC in each run. You can specify the value of the seed by changing the parameter `randomSeed` in the parameter database:

```
pdbSet KMC randomSeed <n>
```

The seed can be set to any value from 0 to 31328.

---

## Boundary Conditions

By default Sentaurus Process KMC uses periodic boundary conditions at the left, right, front, and back sides of the simulation domain. To change these conditions, use the parameters `KMC_PeriodicBC.Y` and `KMC_PeriodicBC.Z`.

By default, the parameter `DebugFlag` is set to 4. With this setting, Sentaurus Process KMC will only use periodic boundary conditions for extended defects such as {311}s and dislocation loops, but it will still use reflective boundary conditions for everything else. This setting reduces the lateral simulation domain for investigating 1D simulations. Even when the lateral simulation domain is comparable to or smaller than the typical length of the extended defect, periodic boundary conditions allow you to obtain meaningful results.

**NOTE** This option must not be used for 3D simulations if there are lateral variations in geometry or profiles.

When Sentaurus Process KMC detects an improper choice of periodic boundary conditions, it changes the periodic conditions:

```
** Warning **
KMC. The material structure is not the same in the plane y=0 and y=ymax.
Periodic boundary conditions for defects have been disabled!
```

The boundary conditions for the bottom are reflective. You can transform them into a sink using the parameter `sinkProbBottom`, which can be defined for any material. For example, to specify that 20% of the incoming positive interstitials should be sunk when reaching the maximum coordinate in silicon, use:

```
pdbSet Silicon KMC I sinkProbBottom IP 0.2
```

It is also possible to define sink boundary conditions for the y- and z-axis, independently of the general *mirror* or *periodic* conditions described below. Similar to the sinks defined in the x-axis, a probability for particles crossing the boundary to be annihilated will be defined. This probability is applied before the general boundary conditions. For example, if a 50% sink is defined for interstitials at the left boundary, 50% of them surviving the sink will be either mirrored or moved to the opposite side to simulate periodicity.

The parameter names for the y-axis are `sinkProbLeft` and `sinkProbRight` and, for the z-axis, they are `sinkProbFront` and `sinkProbBack`.

## Parallelism

You can use several CPUs during a Sentaurus Process KMC simulation using the `math` command:

```
math numThreadsKMC=<i>
```

where `<i>` is the number of threads to launch. When also using MC implantation, the number of threads used by Sentaurus Process KMC overwrites the number of threads used by MC implantation.

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Parallelism

The KMC to PDE "smooth" algorithm (see [Smoothing Out Deatomized Concentrations on page 534](#)) also can work in parallel:

```
math numThreadsDeatomize=<i>
```

Sentaurus Process KMC uses the `parallel` licenses in the same way as Sentaurus Process does. In particular, if no licenses are available, Sentaurus Process KMC will continue in serial or will terminate depending on whether `parallel.license=go.serial` or `parallel.license=go.abort` has been specified by the user in the `math` command.

---

## How Parallelism Works

Sentaurus Process KMC works in parallel by assuming that there is no space anisotropy in the z-direction. This assumption is trivially true for 1D and 2D simulations, and generally false for 3D simulations. Consequently, parallelism is only allowed in simulations that have a 1D or 2D domain in Sentaurus Process (even, when internally, all atomistic simulations are 3D).

The main simulation domain is divided into  $n$  subdomains in the z-direction, where  $n$  is the number of threads to be used. Each subdomain is run as an independent simulation on a different CPU. Then, the boundary conditions selected for the z-boundary are applied to the new  $z_i$ -boundaries. At the end of the simulation (implantation or diffusion), the main domain is recreated as the simple addition of all the subdomains (see [Figure 27](#)). All these 'splits' and 'forks' of the simulation domains are performed automatically and are transparent to users.

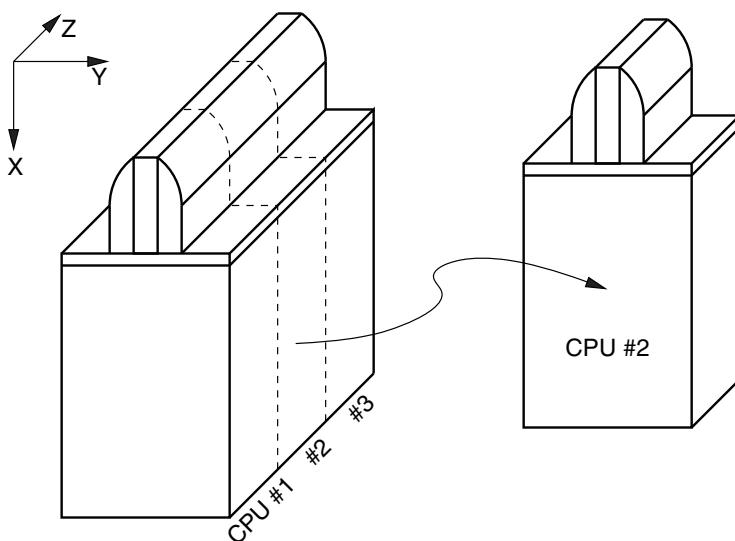


Figure 27 Domain is divided into three subdomains in the z-direction, and each one is processed by a different CPU

When using parallelization, one large parallel simulation domain is run as several smaller domains. At the end of the simulation, the third dimension will be collapsed and averaged to produce a 2D result (third and second dimensions for 1D results). In any case, the subdomains must be large enough to allow an accurate representation of the physics involved in the simulation. In particular, since a minimum surface of  $40 \times 40 \text{ nm}^2$  is recommended, the minimum suggested size for parallel simulations is 40 nm in the y-axis and  $n \times 40$  nm in the z-axis, where  $n$  is the number of threads.

---

## Estimating CPU Time

CPU time and memory required for KMC diffusion simulation are directly proportional to the number of particles in the structure. For a typical 2-GHz machine, Sentaurus Process KMC performs up to 1 million events (jumps) per second. On some 64-bit platforms, the number can reach 2 million events per second.

In equilibrium conditions without implantation damage, concentrations of mobile species are low and events are rare. Therefore, the simulation requires few events to reach the required diffusion time and proceeds quickly.

For transient-enhanced diffusion (TED) after an implantation step, it takes some time to anneal the implantation damage. Depending on the implantation conditions, each implanted ion generates up to  $10^3$  interstitials and vacancies. Each interstitial and vacancy makes up to  $10^5$  jumps before recombining at the surface. This means that it takes approximately 1 second of CPU time to anneal one implanted ion.

**NOTE** The above numbers are estimates only. The CPU speed differs depending on the machine, operating system, and other factors.

Clustering and emission processes take longer internally than diffusion processes (hops) in Sentaurus Process KMC, and similar numbers of simulated clustering or declustering processes may lead to a larger wallclock time.

**NOTE** Using parallelization also changes the time estimate (see [Parallelism on page 385](#)).

**NOTE** Using different *hopping modes* (KMC HoppingMode) also changes the time needed to run the simulation, with longdouble being the fastest mode (see [Hopping Mode on page 417](#)).

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Atomistic Diffusion

## Atomistic Diffusion

The nonlattice KMC method tracks only atoms in defects, while lattice silicon atoms are excluded as shown in [Figure 28](#).

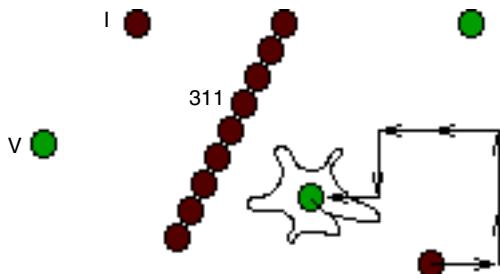


Figure 28 Nonlattice KMC method tracks only atoms in defects; lattice silicon atoms are excluded

In molecular dynamics, all lattice atoms and all defect atoms must be simulated, but in the nonlattice KMC method, only defect atoms are considered. Lattice atoms vibrate with a high frequency because of thermal energy and, occasionally, one of the point defects diffuses and moves to a neighboring position. Since Sentaurus Process KMC uses the nonlattice KMC method, it discards the lattice information and only follows the defect atoms. This greatly affects CPU time, from approximately  $10^{-13}$  s for lattice vibrations to approximately  $10^{-9}$  s for fast diffusing particles. During diffusion, moving particles can be captured by extended defects that emit isolated particles with frequencies orders of magnitude smaller than the frequency of point-defect jumps.

Sentaurus Process KMC takes the input parameters of migration, binding, emission energies, and so on and simulates the frequencies at which these different events occur. Sentaurus Process KMC starts with short time steps, but when the simulation evolves and the fast moving point defects disappear, the average time step automatically changes to adapt to the new situation.

Single particles can move alone or belong to an extended defect, like a {311}:

- For self-silicon point defects, in other words, interstitial and vacancy models, see [Point Defects, Impurities, Dopants, and Impurity-Paired Point Defects on page 408](#).
- For diffusing dopants, see [Impurities on page 411](#).
- For self-silicon extended defects, see [Damage Accumulation Model: Amorphous Pockets on page 428](#) and [Extended Defects on page 438](#).
- For clusters involving dopants, see [Impurity Clusters on page 470](#).

## Units

The units used by Sentaurus Process KMC are:

- Micrometer ( $\mu\text{m}$ ) for length
- Second (s) for time
- Electron volt (eV) for binding energies
- Atoms per  $\text{cm}^3$  for concentrations
- $\text{cm}^2 \text{s}^{-1}$  for diffusivities
- $\text{nm}^3$  for stress activation volumes

**NOTE** These units are standard in atomistic and continuum simulators. Nevertheless, Sentaurus Process KMC internally uses a nonconventional unit to measure frequencies. For consistency with migration prefactors, frequencies are measured in diffusivity units in the input parameter files. However, even for migration prefactors, which are in diffusivity units to easily compare them with experimental numbers, Sentaurus Process KMC must transform them to frequency units in  $\text{s}^{-1}$ . This is performed using the expression  $v = \frac{6D}{\lambda^2}$ , where  $\lambda$  is the average jump distance.

---

## Space Management

Sentaurus Process KMC assumes an orthogonal simulation cell to manage space. The minimum and maximum x-, y-, and z-dimensions (that is, the bounding box) are passed to Sentaurus Process KMC as simulation parameters. Sentaurus Process KMC assumes that the x-axis is the depth of the silicon wafer; whereas, yz is the wafer area.

When Sentaurus Process KMC has the simulation cell size, it splits the space (see [Figure 29 on page 390](#)) using Sentaurus Mesh. This creates an internal grid inside the rectangular simulation boundary box. This grid is used only by Sentaurus Process KMC and is fully isolated from the Sentaurus Process finite-element mesh. These rectangular elements cannot be smaller than the jump distance (0.4 nm). To customize the internal grid, see [Internal Grid on page 382](#).

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Atomistic Diffusion

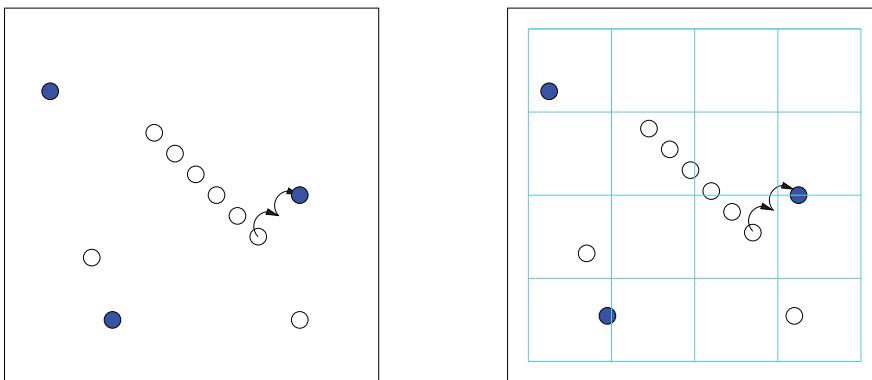


Figure 29 Sentaurus Process KMC divides (*left*) the space into (*right*) small rectangular elements; these elements are used for neighbor search, amorphization, and charge models

Sentaurus Process KMC shows the number of elements in its output:

```
KMC domain (-0.1, 0, 0) to (0.3, 0.16, 0.05) um
```

```
KMC NonUniformTensor. Boxes: 430125
```

```
X=155 (1 - 100) nm
```

```
Y=111 (0.903641 - 1.7048) nm
```

```
Z=25 (2 - 2) nm
```

In the above example, the x-axis minimum cell is 1 nm and the maximum cell is 100 nm. For the y-axis, these values are 0.9 and 1.7 nm, respectively. Finally, all cells have the same size in the z-axis: 2 nm. There are 155 cells in the x-direction, 111 cells in the y-direction, and 25 cells in the z-direction. The total number of elements is 430125.

**NOTE** Memory allocation depends on both the number of internal elements and the number of particles. To modify the number of internal elements, see [Internal Grid on page 382](#).

To add user lines to the simulation, use the `line` command. You also can specify `spacing` in this command. In this case, and in contrast with the nonatomistic mode, there is a minimum size of 0.4 nm between lines. If you specify a very thin spacing, and Sentaurus Mesh tries to add some lines later to better refine a surface, these last lines could be discarded in the KMC mesh only to keep the 0.4 nm limitation. Because refinement box-based criteria will not control mesh spacing precisely, to achieve minimum mesh spacing near the interface, it is recommended to use the `spacing` argument of the `line` command with the following command:

```
pdbSet Grid KMC UseLines 1
```

**NOTE** For tapered structures such as tapered fins, it is advisable to use controlled line spacings along with the PDB setting `pdbSet Grid KMC UseLines 1`. This can be helpful in maintaining a symmetric tensor mesh during atomization and also in avoiding any changes to the tensor-mesh symmetry around the tapered structure due to slight boundary movements.

## Materials and Space

The transfer of materials from Sentaurus Process to Sentaurus Process KMC is straightforward: Each Sentaurus Process KMC element is assigned to a material type. Sentaurus Process KMC creates interfaces whenever two elements are set to different materials, except when instructed not to do so. Consequently, the shape and interfaces assigned by Sentaurus Process KMC depend on the smoothness of the shapes and the fineness of the internal elements (see [Figure 30](#)).

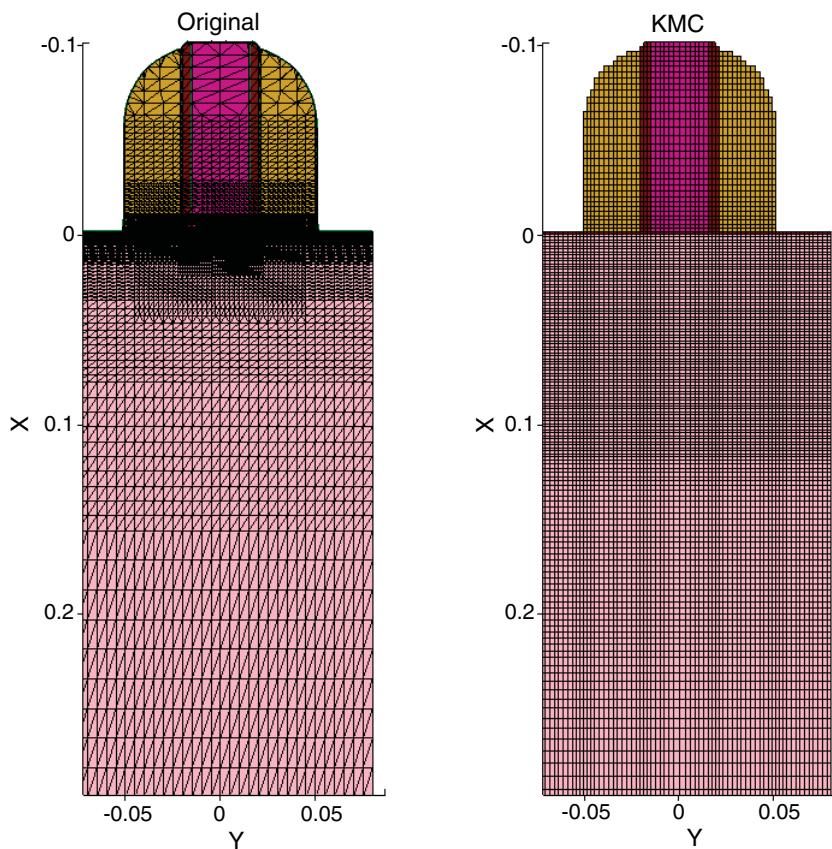


Figure 30 Interface between materials has a Manhattan structure in Sentaurus Process KMC; each element is assigned to a material and elements are always rectangular

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Atomistic Diffusion

The meshing algorithm included in Sentaurus Mesh tries to fit the interfaces using a nonuniform tensor. This fit is perfect when the interfaces are flat and axis aligned, and there are no limitations with the element size due to spacing or very thin features. Since the minimum dimension for an element is 0.4 nm, thinner interfaces will not be accurately represented.

After the material assignment, Sentaurus Process KMC checks that there are no mistakes in the translation by reviewing the original interface elements and checking that there is a corresponding KMC interface associated with them. Whenever this correspondence is not satisfied, Sentaurus Process KMC issues a warning:

```
** Warning **  
KMC. 1.79 percent of the Oxide/PolySilicon interface is lost when translating  
to KMC. Please, review the results carefully.  
... continuing execution
```

**NOTE** In some cases, these warnings may be produced by thin, but negligible, structure shapes. In these cases, the percentage of interface lost is small. When the percentage is significant, these warnings indicate important problems that must be resolved before continuing the simulation.

---

## Supported Material Models

Sentaurus Process KMC supports three material models: `discard`, `simple`, and `full`. These models are selected using PDB parameters. Except for the `discard` model, the `simple` model or the `full` model requires that material properties and all parameters for the material specific to Sentaurus Process KMC must be defined. It would be more convenient to redefine material using the `mater add` command with the `new.like` argument. This enables inheritance of material and interface parameters from the *like* material and respective interfaces.

For materials that are not defined in Sentaurus Process, they must be introduced to Sentaurus Process first with `mater add`. For example, to add a new material called `AnotherSilicon`, which is like silicon:

```
mater add name= AnotherSilicon new.like= Silicon
```

The material `AnotherSilicon` is now also available to Sentaurus Process KMC with the `full` model (inherited from `Silicon`). You can change it to the `simple` model using the following command:

```
pdbSet AnotherSilicon KMC Model simple
```

Alternatively, you can prevent the KMC simulation in `AnotherSilicon` (discarding all particles in this material) by changing to the `discard` model:

```
pdbSet AnotherSilicon KMC Model discard
```

You can assign Amorphous material, but it also is created automatically by changing the crystalline regions during the simulation when the damage reaches an amorphization level (see [Amorphization and Recrystallization on page 450](#)). Therefore, this material is added automatically when its crystalline counterpart is created.

**Table 48** lists the PDB parameters that you must specify for every new material in Sentaurus Process KMC.

Table 48 PDB parameters required for new materials

Parameter	Description
Model	The options are: <ul style="list-style-type: none"> <li>The <code>discard</code> model creates a material empty of particles (for example, gas). All particles introduced in this material are discarded.</li> <li>The <code>simple</code> model includes impurity clusters and simple diffusion of dopants. It does not model Fermi-level dependencies, amorphization, SPER, and extended defects. Oxide and nitride are ‘simple’ materials.</li> <li>The <code>full</code> model allows all models: point defects (interstitials and vacancies), extended defects, impurity clusters, damage accumulation, amorphization, recrystallization, and the Fermi level-dependent diffusivity models (for example, silicon).</li> </ul>
ShortName	This is the short name of the material.
Semiconductor	Boolean parameter that is <code>true</code> for materials where <code>DopingConcentration</code> ( <code>NetActive</code> ) should be computed and stored.
Crystalline	Boolean parameter that is <code>true</code> if the material is crystalline (silicon) or <code>false</code> if it is amorphous (amorphous silicon). It helps determine whether amorphization of the material is possible and is used together with the <code>Equivalent</code> definition. If set to <code>false</code> , a crystalline equivalent definition must be present.
Equivalent	Name of the amorphous/crystalline equivalent. For example, silicon will have amorphous silicon as its equivalent, and the amorphous silicon equivalent is silicon.
Oxide	Specify with <code>true</code> or <code>false</code> whether the material is an oxide or is not an oxide, respectively. This is used for oxidation models. For example, <code>SiOxide</code> and <code>GeOxide</code> have this field as <code>true</code> .
Alloy	Specify if the material can alloy with another material to form binary alloys with corrections to activation energies. Write the alloy material here. For example, for silicon alloying with germanium, write <code>Germanium</code> in the <code>Alloy</code> field of the silicon material.

Defining the `new.like` argument in the `mater` command sets these material definition parameters for the new material to be the same as the `like` material. This also enables copying of the parameters for all the particles in this new material from the `like` material.

The `kmc.shortname` argument can be specified in the `mater` command, which sets the `ShortName` definition for this new material. The `ShortName` can be uniquely defined; otherwise, it will be set as the same as the `like` material.

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Atomistic Diffusion

**NOTE** To minimize the work of defining parameters for a new material, it is advisable to disable the materials (by assigning `discard` to the PDB parameter `<material> KMC Model`) that will not be used, thereby avoiding having to define parameters for the interfaces between those materials and the new one. The dopant parameters in the new material can be inherited from the *like* material, and you can change the parameters in the new materials as required. Parameter inheritance at interfaces complies fully with the properties of *like* inheritance.

**NOTE** Do not use the `ShortName` parameter for new materials, as it is not used and it will be deleted in a future release. This parameter is available for backward compatibility only.

Any other material existing in Sentaurus Process but without the `KMC Model` parameter is mapped as 'Unknown'. The model for this material is `discard`, and all particles inside these materials are discarded and removed. They do not need parameters because they contain no particles to simulate.

---

## Material Alloying

Sentaurus Process KMC allows materials containing an alloying element to be treated in a quasi-atomistic framework. Such an alloying element is specified using the `Alloy` parameter of the material specification. In the following, as an example, it is assumed that the material is silicon and the alloy is germanium (although, this can be reversed, or any pair of materials can be used with "full" modeling).

The quasi-atomistic framework means that alloy particles (Ge) are not created as particles, but they will be taken into account as a field, so as to produce a local concentration. This saves memory and speeds up the concentration. Diffusion of the alloying element is possible using the model specified in [Alloy Diffusion on page 425](#).

Since alloys are treated as a field, alloy distribution depends on the size of the KMC mesh elements. Process steps that change the structure of the domain, such as `etch` or `deposit`, can change mesh-element sizes and, therefore, can affect the redistribution of alloys. Using line commands with the `spacing` argument along with the `pdbSet Grid KMC UseLines 1` setting can help to achieve reproducible distribution of alloy fields after every structure-changing process step. In addition, especially for thin structures, such mesh changes can result in changes in the material in a particular KMC mesh-element location. In such a situation, to deatomize and transfer alloys correctly to the continuum mesh, use the following setting, with values of `<n>` in nm:

```
pdbSet KMC DeAtomize.Search.Dist <n>
```

The inclusion of an alloy changes the bandgap narrowing as specified in [Narrowing due to Presence of an Alloy on page 502](#). Such a model uses a quadratic interpolation to smooth from the band gap of the pure material to the band gap of the pure alloy. Since the positions in the band gap of all particles are scaled with the total band gap, the positions for charged defects are scaled accordingly.

All activation energies for diffusion-, emission-, and activation-related processes are corrected by a term linear on the alloy concentration. If a given mechanism is simulated by following an Arrhenius expression similar to:

$$v = P \exp(-E/k_B T) \quad (680)$$

the mechanisms under an alloy concentration are corrected by a linear term in the activation energy with the concentration of the alloy (Ge):

$$v = P \exp(-(E + \alpha[Ge])/k_B T) \quad (681)$$

The same applies to the formation energies of point defects and the potential energies of impurity clusters. Examples of these corrections are available in [Alloy Effects on page 426](#).

## Point Defects

Sentaurus Process KMC can distinguish different interstitials, depending on the material, using different syntax. The syntax "`I`" refers to an interstitial in the particular material where it is positioned; otherwise, a more concrete notation must be used. For example, in a structure where the first half is Ge and the second half is Si, "`I`" refers to `GeI` in the first half and `SiI` in the second half. While `SiI`, for example, would have the same meaning in the second half as `GeI` in the first half, after diffusing to the first half, it would produce `Si` in the first half.

## Alloying

Sentaurus Process KMC can be used with silicon germanium (SiGe). When using the material `SiGe`, it is important to define the silicon field and the germanium field in the `SiGe` material, to establish a mole fraction. By default, the material will be treated like silicon. It is recommended to use the `MoleFractionFields` command with the `fields.values` argument to set the correct mole fraction of silicon and germanium in the `SiGe` material (see [MoleFractionFields on page 1089](#)). The `fields.values` argument also is found in the `deposit`, `doping`, and `init` commands.

Sentaurus Process KMC also allows an older style of handling alloys used in the materials `Silicon` and `Germanium`, where there is an alloy field in a material. For example, the material `Silicon` has `Ge` specified as an alloy, so that if `Ge` is present in sufficient concentration and if parameter interpolation is switched on by setting `skip.Parameter.Interpolation` to 0 in `Silicon`, it will be considered `SiliconGermanium` without having to change the material.

## Time Management

The main component in Sentaurus Process KMC is an algorithm that sequentially selects the possible random events (such as migration of point defects or emission of extended defects) according to their corresponding frequencies, similar to the Bortz–Kalos–Liebowitz (BKL) algorithm widely used in KMC methods.

[Figure 31](#) illustrates the selection procedure for the atomistic configuration shown in [Figure 28](#) on page 388, consisting of three vacancies (*V*), two interstitials (*I*), and one {311} defect.

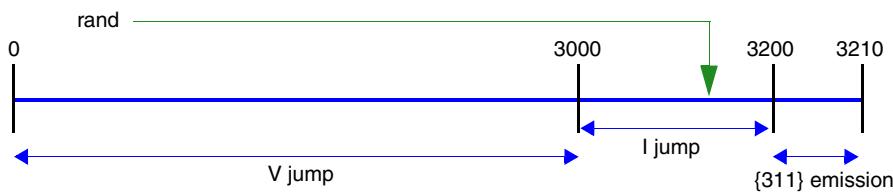


Figure 31 Events are selected according to their rates, which in turn, depend on the current atomistic configuration

Assuming the vacancy and interstitial migration frequencies are  $1000\text{ s}^{-1}$  and  $100\text{ s}^{-1}$ , respectively, and the {311} emission rate is  $10\text{ s}^{-1}$ , to simulate 1 s, you must simulate a total of 3210 events. Consequently, simulating one event corresponds to simulating  $1/3210$  s. This implies that the simulated time step is not fixed, but depends on the particular simulation configuration. In addition, you must choose a *V* with a probability of  $3000/3210$ , and *Is* and {311} defects with probabilities of  $200/3210$  and  $10/3210$ . A random number between 1 and 3210 (or 0 and 3209) is generated. For example, in [Figure 31](#), the number 3147 selects an *I* migration event.

After several migration events, when one interstitial reaches and interacts with a vacancy, the simulator generates an *IV* pair called an *amorphous pocket* (AP) (see [Damage Accumulation Model: Amorphous Pockets](#) on page 428).

The simulation contains two *Vs*, one *Is*, one *IV*, and one {311}. You can assume the *IV* pair will recombine with a frequency of  $500\text{ s}^{-1}$ . The new random number will be between 1 and  $2000 + 100 + 500 + 10 = 2610$ . Consequently, the time step will be  $1/2610$  s. If the *IV* recombination event is chosen and this *IV* pair is annihilated, the new simulation contains only two *Vs*, one *I*, and one {311}, and the following time step is  $1/2110$  s.

**NOTE** The time step is not a fixed quantity in Sentaurus Process KMC, but it depends on the state of the simulation.

The current time step depends on the:

- Number of particles in the simulator.
- Frequency of the events associated with the particles, or defects, or both.

These frequencies depend on the:

- Type of event.
- Arrhenius plot associated with the event.
- Temperature.

---

## Simulation and CPU Times

The time needed to complete a simulation depends on several factors:

- How fast the computer simulates one event
- How many events need to be simulated
- The hopping mode chosen
- The presence of lattice KMC models (for SPER and epitaxial deposition)
- Whether you use parallel capabilities

The number of events to be simulated is inverse to the average time step (which changes during the simulation, as explained above). The speed at which the simulator processes the events depends on the types of the simulated events.

Migration events usually are simulated rapidly. Simulations involving changes in the electronic concentration or temperature or both are much slower because updating the dependencies with the temperature and the Fermi level takes extra time. Generally, the smaller the simulation, the shorter the time.

In simulations with implantations, Sentaurus MC also adds time to the simulation while computing the cascades. In amorphizing conditions, the Sentaurus Process KMC amorphous model requires extra time to smooth out the damage and to create amorphous layers. Finally, simulations with strong gradients in the electronic concentration need more charge updates, which take extra time.

During oxidation, several remeshings must be performed to update the Sentaurus Process KMC structure to the new Sentaurus Process oxide thickness, consuming extra time.

Finally, the hopping mode allows you to choose whether long hops or double hops are allowed, thereby speeding up the simulation. Both are switched on by default (see [Hopping Mode on page 417](#)).

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Atomistic Diffusion

**NOTE** You can estimate the time needed for a simulation by running a small simulation and assuming the CPU time is proportional to the number of particles, which is proportional to the surface area.

Sentaurus Process KMC shows the status of the current simulation, printing log messages each time the temperature changes during a temperature ramp, or whenever there is a new *snapshot* (see [Snapshots on page 399](#)).

An example of a log message is:

```
Reaction :      31s   to      63s   step   :      32s   temp: 950.0C
Mechanics:     31s   to      63s   step   :      32s   temp: 950.0C
Diffusion:     31s   to      63s   step (d):  32s   temp: 950.0C
KMC: Time(s)  Temp(C)    Events Events/s Average step(s) %Done
        46.416    950.01  3600728007  1877077   4.749174e-08  7.74% (36% V)
Reaction :      1.05min to    2.117min step   :      1.067min temp: 950.0C
Mechanics:     1.05min to    2.117min step   :      1.067min temp: 950.0C
Diffusion:     1.05min to    2.117min step (d):  1.067min temp: 950.0C
KMC: Time(s)  Temp(C)    Events Events/s Average step(s) %Done
        100.000   950.01  4742533558  1865695   4.692958e-08  16.67% (33% V)
Reaction :      2.117min to    4.25min step   :      2.133min temp: 950.0C
Mechanics:     2.117min to    4.25min step   :      2.133min temp: 950.0C
Diffusion:     2.117min to    4.25min step (d):  2.133min temp: 950.0C
KMC: Time(s)  Temp(C)    Events Events/s Average step(s) %Done
        215.444   950.01  6881748852  1868310   5.396525e-08  35.91% (34% I)
Reaction :      4.25min to    7.125min step   :      2.875min temp: 950.0C
Mechanics:     4.25min to    7.125min step   :      2.875min temp: 950.0C
Diffusion:     4.25min to    7.125min step (d):  2.875min temp: 950.0C
Reaction :      7.125min to    10min step   :      2.875min temp: 950.0C
Mechanics:     7.125min to    10min step   :      2.875min temp: 950.0C
Diffusion:     7.125min to    10min step (d):  2.875min temp: 950.0C
KMC: Time(s)  Temp(C)    Events Events/s Average step(s) %Done
        464.159   950.01  11927967061  1864825   4.928753e-08  77.36% (35% I)

Elapsed time for diffuse 7.8672e+03s
       600.000   950.01  14721335445  1882323   4.862968e-08 100.00% (35% I)
```

It is easy to identify the log immediately after the Diffusion statement because KMC: starts the line. In the above example, the total simulated (annealed) time is 600 s. The (current) temperature is 950°C. A total of  $1.4 \times 10^{10}$  events has been simulated so far, and the simulator processed 1.9 million events each CPU second. The averaged time step was  $4.9 \times 10^{-8}$  s. Finally, Sentaurus Process KMC writes the particle with the biggest percentage of diffusion jumps. In the example, the diffusion of the neutral interstitial (I) has taken 33% to 36% of the total diffused particles.

This information may change from one simulation to another, and also at different times during the same simulation. The events per second and the average step statistics are recomputed between sentences.

## Parallelism and CPU Time

[Table 49](#) lists the CPU times that can be expected when running on different numbers of threads. However, the exact time depends on the particular simulation.

Table 49 Approximate CPU times when using multiple threads

Number of independent threads	Approximate time	Improvement
1	S	1x
2	S/2.3	2.3x
4	S/4.8	4.8x
8	S/8	8x
12	S/9.5	9.5x
16	S/10.5	10.5x

The total simulation time is superlinear for  $n < 8$  and starts saturating for  $n \geq 12$ . The reason for being superlinear for a small number of threads is that the CPU time depends superlinearly on size. Consequently, simulating a size of  $XYZ/n$  takes less CPU time than  $S/n$ . Nevertheless, as  $n$  increases, different mechanisms (such as the waiting time of threads to be synchronized) conspire to degrade the total simulation time.

## Snapshots

A snapshot is an interruption to the usual Sentaurus Process KMC simulation flow so as to print the status of the simulation and to allow you to run a customizable Tcl command (see [Movie on page 400](#)). To control these interruptions, set the parameters listed in [Table 50](#).

Table 50 PDB parameters required for snapshots

Parameter	Description
Decade <n>	Sets how many snapshots will be generated per decade. Specify 0 to disable it.
InitOutputTime <n>	No snapshots per decade are generated when the simulated time is smaller than <n>.
maxSnapshots <n>	Maximum number of snapshots to be stored. After this limit is reached, the oldest snapshots are deleted to make space for the new ones.

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Atomistic Diffusion

For example:

```
pdbSet KMC Decade 2
```

produces two snapshots per decade, as in:

Time (s)	Temp (C)	Events	Events/s	Average step (s)	%Done
0.000	26.85	0			
548.138	700.00	1	5.481385e+02	5.481385e+02	0.05% (35% I)
1492.073	700.00	5	2.359835e+02	2.359835e+02	0.15% (33% I)
3639.863	700.00	7867	2.731862e-01	2.731862e-01	0.36% (35% I)
10130.431	700.00	14553	9.707701e-01	9.707701e-01	1.01% (35% I)
31902.727	700.00	35862	1.021742e+00	1.021742e+00	3.19% (36% I)
100030.228	700.00	205821	169959	4.008467e-01	10.00% (35% I)
317268.817	700.00	668173		4.698554e-01	31.73% (34% I)
1000000.000	700.00	1754838	1086665	6.282812e-01	100.00% (35% I)

## Movie

The Sentaurus Process KMC Movie command is similar to the Sentaurus Process Movie command and executes the contents of the parameter KMC Movie any time a new snapshot is generated. You can use this command interactively to obtain information about the simulation, to add data to the TDR file of Sentaurus Process KMC, and so on.

For example, it can be used to add concentration information and the positions of particles to the TDR file during the simulation:

```
pdbSet KMC Movie {kmc extract tdrAdd concentrations defects}
```

To plot the evolution of damage while the simulation is still running, use:

```
pdbSet KMC Movie {
    kmc deatomize name=ITotal; sel z=log(ITotal+1); plot.1d label=I clear;
    kmc deatomize name=VTotal; sel z=log(VTotal+1); plot.1d label=V !clear
}
```

---

## Time Internal Representation and Limitations

There are no internal limits for the frequencies used in Sentaurus Process KMC. Nevertheless, very high frequencies (typically produced by small migration energies) can lead to slow simulations.

## Particles

Particles are represented in Sentaurus Process KMC with three spatial coordinates (x, y, z) and two labels:

- The *particle* type identifies the species, the charge state, and the role of the particle in the simulation.
  - The *defect* type indicates when the particles are agglomerated with others or when they stand alone.
- 

## Particle Types

To list the standard particles currently defined for Sentaurus Process KMC, at the command prompt, type:

```
sprocess> kmc partictypes
I V B As C F In O P Sb N H IMM IM IP IPP VMMM VMM VM VP VPP VPPP Asi AsiP AsV
AsVP AsVM Bi BiP Bim Ci FV FI Ini IniM InV InVM Pi PiP PV PVM PVP Sbi SbiP SbV
SbVP SbVM Ge Gei Si Sii
```

Dopants are user defined in Sentaurus Process KMC, while interstitials and vacancies are fixed and cannot be customized. [Table 51](#) lists the interstitials and vacancies defined in Sentaurus Process KMC.

Table 51 Interstitials and vacancies defined in Sentaurus Process KMC

Interstitial or vacancy	Description
I	Silicon self interstitial–neutral
IMM	Silicon self interstitial–double negative
IM	Silicon self interstitial–negative
IP	Silicon self interstitial–positive
IPP	Silicon self interstitial–double positive
V	Vacancy–neutral
VMMM	Vacancy–triple negative
VMM	Vacancy–double negative
VM	Vacancy–negative
VP	Vacancy–positive

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Particles

Table 51 Interstitials and vacancies defined in Sentaurus Process KMC

Interstitial or vacancy	Description
VPP	Vacancy–double positive
VPPP	Vacancy–triple positive

The dopants are defined in the parameter database. By default, particles for As, B, P, In, C, F, N, Nn ( $N_2$ ), H, and Sb are defined. For example, [Table 52](#) lists the default particles for As, B, and P.

Table 52 Default particles for As, B, and P

Particle	Description
As	Substitutional arsenic–positive
Asi	Interstitial arsenic–neutral
AsiP	Interstitial arsenic–positive
AsV	Vacancy arsenic–neutral
AsVM	Vacancy arsenic–negative
AsVP	Vacancy arsenic–positive
B	Substitutional boron–negative
Bi	Interstitial boron–neutral
BiM	Interstitial boron–negative
BiP	Interstitial boron–positive
P	Substitutional phosphorus–positive
Pi	Interstitial phosphorus–neutral
PiP	Interstitial phosphorus–positive
PV	Vacancy phosphorus–neutral
PVM	Vacancy phosphorus–negative
PVP	Vacancy phosphorus–positive

**NOTE** Since P at the end of the name means *positive*, to specify a cluster containing phosphorus, P can never be used at the end of a name. This means that AsiP is an arsenic–interstitial positive, while PAsi is a phosphorus–arsenic–interstitial cluster. Similarly, AsP will be interpreted as *arsenic positive*, while PAs is phosphorus–arsenic.

**NOTE** [Table 51 on page 401](#) and [Table 52 on page 402](#) list the most commonly used particles, but the list is not exhaustive. An exhaustive list contains all point defects (*I*s and *V*s) with charges from  $-3$  to  $+3$ , and all impurity pairs with charges from  $-2$  to  $+2$ .

## Particles in Models

The dopants allowed in the simulation are defined in the parameter database under the label `KMC Impurities`. The parameter database lists the impurity name, the charge, and a Boolean parameter indicating whether the particle is allowed in the Sentaurus Process KMC simulation.

The particle name and the charge must be delimited by a comma without spaces. For example, in the case of arsenic and boron:

```
pdbSet KMC Impurities As,1    true
      pdbSet KMC Impurities B,-1   true
```

When the dopant type has been defined, the paired particles (particles with *I* or *V*) can be defined in `KMC Pairs`. The definitions are a string containing the name of the pair, the name of the dopant, the type of pair (*I* or *V*), and the charge. These fields are separated with commas. Finally, a Boolean parameter instructs Sentaurus Process KMC to take the particle into account.

For arsenic and boron:

```
pdbSet KMC Pairs Asi,As,I,0    true
      pdbSet KMC Pairs AsiP,As,I,1   true
      pdbSet KMC Pairs AsV,As,V,0    true
      pdbSet KMC Pairs AsVP,As,V,1   true
      pdbSet KMC Pairs AsVM,As,V,-1  true
      pdbSet KMC Pairs BV,B,V,0     false
      pdbSet KMC Pairs Bi,B,I,0     true
      pdbSet KMC Pairs Bi,B,I,0     true
      pdbSet KMC Pairs BiP,B,I,0    true
      pdbSet KMC Pairs BIM,B,I,-1   true
```

In the above example, the boron–vacancy particle is not defined (it is set to `false`). A particle is not defined when it does not appear in the `Pairs` list, or when its Boolean value is `false`.

The following rules must be followed when defining particles:

- The dopants used in the definitions of `Pairs` must exist in the list of impurities.
- A charge  $n$  can only be defined when a charge  $n - 1$  or  $n + 1$  is already defined, except for pairs with the same charge states as their dopants.
- Charge states without possible pairing reactions cannot be defined.

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Particles

- The charge must be -1, 0, or +1.
- Pairs with a neutral state and with the charge of its dopant must always be defined.

For example, when  $\text{As}^+$  is defined as an impurity,  $\text{AsV}^+$  can be defined. The existence of  $\text{AsV}^+$  allows you to define  $\text{AsV}^0$  and  $\text{AsV}^-$ .  $\text{AsV}^{--}$  cannot be defined (no charge -2). For  $\text{B}^-$ , you can define  $\text{B}_i^-$ ,  $\text{B}_i^0$ , and  $\text{B}_i^+$ .

### Aliases of Particle Names

Aliases of particle names are defined using `KMC aliases`, which is a list of particle names and alternative names separated by commas. These aliases are used only when Sentaurus Process KMC tries to map a name as a particle or a defect. For example, if there is an alias such as:

```
Bi BoronInt,BI
```

the following commands are identical:

```
kmc present defectname=Bi  
kmc present defectname=BI
```

In addition, the following commands create fields with different names, but the atomized particle is the same (`Bi`):

```
sel z=1e19 name=Bi  
sel z=1e19 name=BI  
sel z=1e19 name=BoronInt
```

### Colors of Particles

You can change the default visualization color for the atomistic representation of particles and defects in Sentaurus Visual, or add new colors to existing particles and defects.

You can return the list of colors using `KMC Colors`, and the list is an array of particle names and colors in #rrggbbaa format (red, green, blue).

### Particles and Parameters

New particles need new parameters. For every impurity specified in `Impurities`, a new file must be created for each material folder and surface. The name of these files is obtained using the `alias` command with the name of the Sentaurus Process KMC impurity as a parameter:

```
sprocess> alias B  
Boron
```

**Table 53** lists the parameters required for materials defined to use the simple model.

Table 53 Nonsilicon material parameters

Parameter	Description
Dm, Em	Diffusion parameters.
VD, VF	Activation volumes for stress.
sinkProbTop, sinkProbBottom, sinkProbLeft, sinkProbRight, sinkProbFront, sinkProbBack	Boundary conditions.
Implement.Complex	Parameters for clustering.
ReactionsPointDefect, ReactionsCluster	Binary interactions.

When amorphous materials (where the best example is amorphous silicon) use the dangling bond model (see [Indirect Diffusion Model on page 453](#)), the parameters in both **Table 53** and **Table 54** are required.

Table 54 Extra parameters for amorphous materials

Parameter	Description
EmGe, EfGe	Germanium correction to migration energies.
gamma	Coefficient for dangling bond creation.
Db, Eb	Binding prefactor and energy.

**Table 55** lists the parameters used on interfaces.

Table 55 Parameters used on interfaces

Parameter	Description
EBarrier_?, Eb_?	Interface binding energies for dopants, where ? denotes the material. Gas for gas, Silicon for silicon, Oxide for oxide, Nitride for nitride, PolySilicon for polysilicon, AmorphousSilicon for amorphous silicon material, and so on for any material with the full model.
Db.Surf	Surface emission prefactor for dopants.
EMax.Surf, C0Max.Surf	Maximum number of particles trapped at the surface.
Factor.Max.Surf, Exp.Max.Surf	Controls segregation depending on the existing impurity at the interface.
Evaporation.Surf	Probability to evaporate (annihilate).
VF_?	Activation volume for stress, where ? denotes the material.
Pref.GrowthDeposit, Ener.GrowthDeposit	Controls redistribution of dopants during growth, such as silicidation.

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Particles

[Table 56](#) lists the parameters required for materials defined to use the full model.

Table 56 Parameters for full model

Parameter	Description
Dm, Em	Diffusivities.
Db, Eb	Binding prefactors and energies.
VD, VF	Activation volumes for stress.
e0	Electronic levels.
EfGe, EmGe	Corrections for germanium.
C0.Epi.Max.Active, E.Epi.Max.Active, Epi.Deposit.Active, Epi.Deposit.Complex	Controls activation and clustering of dopants during epitaxy.
Pref.RecrystDeposit, Ener.RecrystDeposit, C0.Recryst.Max.Active, E.Recryst, E.Recryst.Exponent, E.Recryst.Max.Active, e0.Complex, Recryst.Deposit.Active, Recryst.Deposit.Complex, Recryst.Deposit.Threshold, Recryst.Max.Size, Recryst.Max.Total	SPER model (recrystallization).
sinkProbTop, sinkProbBottom, sinkProbLeft, sinkProbRight, sinkProbFront, sinkProbBack	Boundary conditions.
ReactionsPointDefect, ReactionsCluster, ReactionsClusterI, ReactionsClusterV, ReactionsClusterIV, ReactionsLoop, ReactionsVoid, Reactions311	Binary interactions.

Finally, amorphous, simple and full materials allow the definition of impurity clusters. These clusters are defined using the parameters listed in [Table 57](#).

Table 57 Parameters used for impurity clusters

Parameter	Description
Implement.Complex	Whether a cluster exists or not.
Etotal.Complex	Cluster potential energy.
e0.Complex	Cluster charge.
VF.Complex	Stress dependency.
CaptVol.Complex	Cluster capture volume used for emission.
D0.Cluster	Cluster emission prefactors.
EbarrierDopant.Complex, EbarrierIV.Complex	Cluster emission barriers.
Dm.Complex, Em.Complex	Cluster migration parameters

For further explanations on these parameters, see the comments in the parameter database and the model descriptions.

## Undefining Particles

A particle can be *undefined* by deleting its definition in the parameter database or by setting its Boolean to `false`. If an impurity is undefined, Sentaurus Process KMC also undefines all its pairs.

For example, to undefine indium in a simulation, use:

```
pdbSet KMC Impurities In,-1 false
```

To undefine only boron–interstitials with a positive charge, use:

```
pdbSet KMC Pairs BiP,B,I,1 false
```

**NOTE** Undefining particles that will not be used in a simulation saves some memory and CPU time. If an undefined dopant is used (for example, it is implanted or introduced with the `select` command), it generates an error message.

## Defect Types

To list the defects implemented in Sentaurus Process KMC (see [Table 58](#)), on the command line, type:

```
sprocess> kmc defecttypes
```

Table 58 Defects implemented in Sentaurus Process KMC

Defect	Description
Amorphous	Amorphous region inside the crystalline silicon. Only <i>I</i> , <i>V</i> , impurity clusters, and dopants are allowed. See <a href="#">Amorphization and Recrystallization on page 450</a> .
AmorphousPocket	Disordered agglomeration of <i>Is</i> and <i>Vs</i> (damage). Only <i>I</i> and <i>V</i> particle types are allowed. See <a href="#">Damage Accumulation Model: Amorphous Pockets on page 428</a> .
ImpurityCluster	Impurity clusters. Agglomeration of dopants with <i>Is</i> or <i>Vs</i> . See <a href="#">Impurity Clusters on page 470</a> .
Interface	Dopants trapped in the interfaces (for example, Si–SiO <sub>2</sub> interface). See <a href="#">Interfaces and Surfaces on page 506</a> .
LatticeAtom	Atom in the silicon lattice used for SPER or epitaxial deposition. See <a href="#">LKMC: Fully Atomistic Modeling of Solid Phase Epitaxial Regrowth on page 458</a> .

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Point Defects, Impurities, Dopants, and Impurity-Paired Point Defects

Table 58 Defects implemented in Sentaurus Process KMC

Defect	Description
Loop	Dislocation loops. Extended <i>Is</i> defect. Only <i>Is</i> are allowed. See <a href="#">Dislocation Loops on page 442</a> .
PointDefect, PD	Single particles (IMM, IM, I, IP, IPP, VMM, VM, V, VP, VPP, AS, and B) or paired ones (Asi, AsiP, AsVM, AsV, AsVP, BiM, Bi, and BiP) that do not belong to any extended defect or particle agglomeration; in other words, impurities, dopants, and impurity-paired point defects.
Rejected	A particle coming from MC implantation that is determined to be in a material that does not support the particle. For example, a point defect in a simple material such as oxide.
ThreeOneOne	{311} rod-like extended defects. Only <i>Is</i> are allowed. See <a href="#">{311} Defects (ThreeOneOne) on page 438</a> .
TwinDefect	Can be formed during SPER if the twin defect model is switched on. See <a href="#">Defect Generation During SPER on page 464</a> .
Void	Vacancy clusters with spherical shape. Only Vs are allowed. See <a href="#">Voids on page 447</a> .

**NOTE** Not all possibilities of particle and defect types are allowed. Some particle types, such as paired ones (Asi, BiM), are only allowed as PointDefect. Others such as As or B can stand alone (PointDefect), can be trapped in interfaces (Interface), or can belong to an impurity cluster (ImpurityCluster). Neutral interstitials, for example, can stand alone (PointDefect) and can be in damaged clusters (AmorphousPocket), {311} defects (ThreeOneOne), or dislocation loops (Loop). Single particles can be mobile point defects (that is, interstitials and vacancies), immobile impurity atoms (like substitutional boron and arsenic), and also mobile impurity-defect pairs such as Bi or AsV. All are considered PointDefect.

---

## Point Defects, Impurities, Dopants, and Impurity-Paired Point Defects

This section describes the models related to the creation, diffusion, or interaction of various point defects considered in KMC simulations. It also describes the parameters that enable users to add their own interactions or to control the interactions of existing point defects.

## Interstitials and Vacancies

Interstitials and vacancies in Sentaurus Process KMC perform a diffusion event in each axis  $j$  (x, y, and z) at a frequency given by the expression:

$$v_m^j = \frac{v_{0,m}}{3} \cdot \exp\left(-\left(E_m + \sigma'_j \Delta V_{par} + \sum_{i \neq j} (\sigma'_i \Delta V_{ort}) + \Delta E_m(Ge)\right)/(k_B T)\right) \quad (682)$$

where:

- $v_m^j$  is the jump frequency for the axis  $j$ .
- $v_{0,m}$  is the prefactor.
- $E_m$  is the migration energy.
- $\sigma'_i$  are the principal stresses (the stresses in the coordinate system where all the stress tensor nondiagonal components are null).
- $\Delta V_{par}$  is the activation volume for stress-parallel diffusion.
- $\Delta V_{ort}$  is the activation volume for stress-perpendicular diffusion.
- $\Delta E_m(Ge) = \alpha_m[Ge]$  is the correction due to germanium concentration.

These parameters are called `Dm` (prefactor), `Em` (migration energy), `VD` (activation volumes), and `EmGe` (for  $\alpha_m$ ) in the parameter database. They are defined only in the `full` model materials:

```
sprocess> pdbGet Si KMC I Dm
IMM 5e-2
IM 5e-2
I 5e-2
IP 5e-2
IPP 5e-2
sprocess> pdbGet Si KMC I Em
IMM 0.8
IM 0.8
I 0.8
IP 0.8
IPP 0.8
sprocess> pdbGet Si KMC I VD
IMM 0,0
IM 0,0
I 0,0
IP 0,0
IPP 0,0
sprocess> pdbGet Si KMC I EmGe
0
```

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Point Defects, Impurities, Dopants, and Impurity-Paired Point Defects

The activation volumes for parallel and perpendicular diffusion are separated by a comma (no spaces) in VD.

The stresses  $\sigma_{ij}$  are produced by Sentaurus Process and imported by Sentaurus Process KMC. This stress tensor is diagonalized to obtain the principal stresses  $\sigma'_i$ . The directions x, y, and z used in the equation refer to the system in which the stress tensor is diagonal.

**NOTE** You can calibrate these parameters if necessary to change the point-defect diffusivity and the diffusion coefficient (DC) product.

Sentaurus Process KMC simulates point-defect migration, modifying the particle coordinates in the orthogonal directions a fixed distance, called  $\lambda$ , which corresponds to the second neighbor's distance in the silicon lattice (0.384 nm). The value of  $\lambda$  can vary spatially (as explained in [Hopping Mode on page 417](#)).

After each diffusion event, the charge state of the point defect is updated according to the new local Fermi level (see [Fermi-Level Effects: Charge Model on page 488](#) and [Updating Charge States on page 495](#)). Whenever a jumping point defect encounters another particle, defect, or interface, the jumping point defect interacts according to the specific situation.

The allowed interactions depend on the:

- Incoming species: For example, substitutional boron plus interstitial (B + I) is allowed, and the incoming species forms a boron–interstitial. Boron plus vacancy is not allowed. This interaction can be enabled or disabled in the parameter database.
- Energetics: Sentaurus Process KMC allows interactions for {311} defects, dislocation loops, and pairing because the binding energies are greater than 0. For impurity clusters, if the reaction is unfavorable, the newly formed defect breaks up and dissolves into the original components or is rejected before reacting.
- Charge states: Interactions between repulsive species are forbidden, except for the ‘percolation’ model (see [Percolation on page 475](#)).

Mobile particles can interact with other mobile particles or with the particles belonging to extended defects, whenever they enter the capture radius of the other particle or defect (see [Figure 32 on page 411](#)). The capture radius of a mobile particle is  $\lambda$ , assumed to be the same as the jumping distance. For extended defects, the capture volume is the sum of the capture volumes of its constituent particles. Mobile particles can interact with surfaces or interfaces (see [Interfaces and Surfaces on page 506](#)).

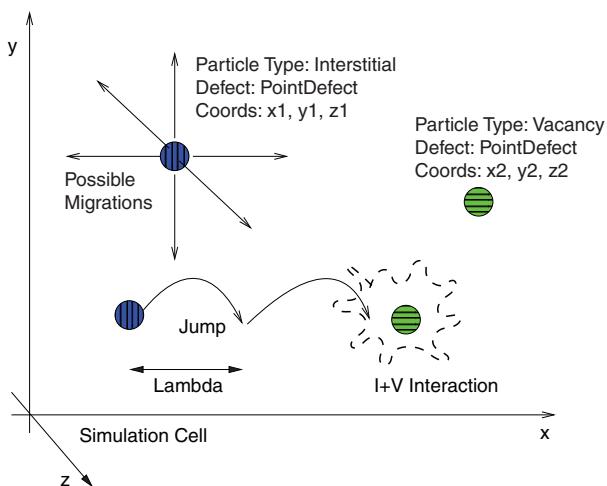


Figure 32 Point defects diffuse by jumping a distance  $\lambda$  in any orthogonal direction and can interact with neighbor particles

## Impurities

Isolated impurities in Sentaurus Process KMC can be in a substitutional state or can be paired with interstitials or vacancies. Substitutional impurities are electrically active and typically immobile. The acceptor and donor impurities (group III and group V of the periodic table, respectively) can move in silicon only by pairing with an interstitial or a vacancy, as shown in the literature [4][5][6][7][8]. Other impurities, such as fluorine, may diffuse without the aid of an extra I or V (see [Impurities Diffusing Without Pairing on page 521](#)).

Impurity atoms are modeled like interstitials or vacancies. They have a position, a defect type, and a particle type. The defect type is `PointDefect`, and the particle type characterizes the species, the charge state, and the presence of a paired I or V. For example, `BiM` indicates a negatively charged boron paired with an interstitial.

**NOTE** Sentaurus Process KMC assumes interstitial particles and substitutional particles paired with an interstitial have the same configuration. For example, `Bi` is the same as `IB` or `BI`, and there is only one position (three coordinates) for it.

Paired impurities can perform different events:

- Diffusion
- Breakup of the impurity–defect pair
- Percolation

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Point Defects, Impurities, Dopants, and Impurity-Paired Point Defects



Figure 33 Impurity pairs can diffuse or break up into a substitutional plus an interstitial or a vacancy

**NOTE** Fluorine is modeled as an interstitial particle (in the default parameters, not in Advanced Calibration). Consequently, fluorine diffuses without pairing. See [Impurities Diffusing Without Pairing on page 521](#).

## Diffusion

A diffusion event is defined as for point defects (see [Eq. 682, p. 409](#)). Nevertheless, the equation defines an *instant* diffusivity that is different from the *effective* diffusivity. Effective diffusivity measured in experiments involves a large number of microscopic migration steps and long times. Microscopically, dopants diffuse using the kick-out mechanism. For example, when an interstitial reacts with a substitutional boron, a boron–interstitial pair is generated:  $B + I \rightarrow B_i$ . In contrast with the boron in a substitutional position, the generated pair is mobile. Then,  $B_i$  begins to diffuse, using the diffusivity parameters specified in [Eq. 682](#). After some time, the interstitial boron breaks up, releasing the interstitial. This boron will not move until a new incoming  $I$  reacts with it. Consequently, the macroscopic diffusivity is related not only with the boron–interstitial diffusivity, but also with its breakup frequency as:

$$D^{\text{eff}}(B) = D_0^{\text{eff}}(B) \exp\left(-\frac{E_{\text{diff}}(B)}{k_B T}\right) \quad (683)$$

where:

- $D_0^{\text{eff}}(B)$  depends on the Bi and I migration prefactors and on the Bi breakup prefactor.
- $E_{\text{diff}}(B)$  is related to the Bi microscopic migration energy  $E_m(B_i)$ , the formation energy of an interstitial  $E_f(I)$ , and the Bi binding energy  $E_b(B_i)$  (assuming there is no stress or corrections):

$$E_{\text{diff}}(B) = E_m(B_i) + E_f(I) - E_b(B_i) \quad (684)$$

Finally, the total boron diffusivity is given as the sum of the contribution of all mobile species. For boron–interstitial, and assuming there are three mobile species (negative, neutral, and positive):

$$D(B) = D(B_i^-) \frac{[B_i^-]}{[B^-]} + D(B_i^0) \frac{[B_i^0]}{[B^-]} + D(B_i^+) \frac{[B_i^+]}{[B^-]} \quad (685)$$

where  $D(B_i^x)$  represents the microscopic pair diffusivity of charge  $x$ .

## Breakup

A breakup event for an interstitial–impurity pair can be described as:



where  $A_i$  is an interstitial–impurity pair,  $A_s$  is a substitutional impurity atom, and  $I$  is an interstitial silicon atom.

This breakup event happens with a frequency given by:

$$\nu_{bk} = \nu_{0,bk} \cdot \exp(-E_{bk}/(k_B T)) \sum_i^{x,y,z} \exp(-\Delta E_m^i/(k_B T)) \quad (687)$$

where  $\nu_{0,bk}$  is the prefactor and  $E_{bk}$  is the activation energy, defined as the binding energy plus the migration energy of the emitted species and the SiGe and stress corrections:

$$E_{bk}(A_i) = E_b(A_i) + E_m(I) + P(\Delta V_f(I) + \Delta V_f(A) - \Delta V_f(A_i)) + [Ge](\alpha_f(I) + \alpha_f(A) - \alpha_f(A_i)) \quad (688)$$

where:

- $P = \left(-\frac{1}{3}\right)(\sigma'_x + \sigma'_y + \sigma'_z)$  is the hydrostatic pressure, computed as the mean value of the principal stresses.
- $\Delta V_f$  are the activation volumes for the formation energies.
- $[Ge]$  is the germanium concentration.
- $\alpha_f$  accounts for the variation of the formation energy with the germanium concentration.

The corrections to the migration energies induced by the stress and SiGe are (as explained in [Interstitials and Vacancies on page 409](#)):

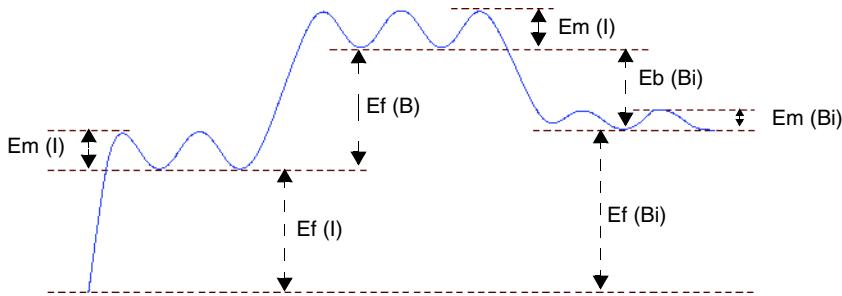
$$\Delta E_m^i = \sigma'_j \Delta V_{par} + \alpha_m [Ge] + \sum_{i \neq j} (\sigma'_i \Delta V_{ort}) \quad (689)$$

## 5: Atomistic Kinetic Monte Carlo Diffusion

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Sentaurus Process KMC assumes that the activation volume and the SiGe variation for the formation energy do not depend on the charge. All the charge states of the same species share the same activation volume and SiGe dependencies for the formation energy.

[Figure 34](#) shows the energies for boron involved in this mechanism.



**Figure 34** Energies involved in the kick-out mechanism for  $B^- + I^0 = Bi^-$ . Migration energy of the interstitials and boron–interstitial are specified in the parameter database as  $Em$ . The binding energies are  $Eb$ , and the  $I$  formation energy is specified as  $Ef$ . The formation energy for dopants in pure silicon is assumed to be 0 because the dopants are already in the simulation; the dopants are not created by the system.

It is easy to deduce that a change in the formation energies due to stress and SiGe will change the binding energy as:

$$\Delta E_b(B_i) = \Delta E_f(I) + \Delta E_f(B) - \Delta E_f(B_i) \quad (690)$$

## Percolation

In a percolation event, an impurity can react with any other defect in its neighborhood without the need for diffusion. In this aspect, it can simulate the reactions that occur through distortions in the lattice but without the need for the migration of particles. The neighborhood of the particle is defined in the same way as for diffusing point defects.

The percolation rate, that is, the frequency at which the particle attempts to interact with any valid defect in its neighborhood, is defined as:

$$v_{\text{per}} = P_{\text{per}} \exp\left(-\frac{E_{\text{per}}}{k_B T}\right) \quad (691)$$

where  $P$  and  $E$  are the prefactors for percolation, specified as input parameters. Percolation only applies to substitutional dopants or impurities. It can provide an extra mechanism for dopant deactivation at very high concentrations.

## Parameters

The dopant diffusion parameters are stored in the parameter database for each material and dopant, under the names `Dm`, `Em` for diffusivities, and `Db`, `Eb` for binding energies. `Dm` and `Db` are prefactors, and `Em` and `Eb` are energies. The activation volumes for the formation energies have the name `VF` and  $\alpha_f$  is called `EfGe`. The prefactor and the activation energy for percolation are called `D0.Percolation` and `E0.Percolation`, respectively.

The following parameters can be changed:

```
pdbSet <material> KMC <Dopant> Dm <particle type> <value>
pdbSet <material> KMC <Dopant> Em <particle type> <value>
pdbSet <material> KMC <Dopant> Db <particle type> <value>
pdbSet <material> KMC <Dopant> Eb <particle type> <value>
pdbSet <material> KMC <Dopant> VF <particle type> <value>
pdbSet <material> KMC <Dopant> VD <particle type> <value>,<value>
pdbSet <material> KMC <Dopant> EfGe <particle type> <value>
pdbSet <material> KMC <Dopant> D0.Percolation <value>
pdbSet <material> KMC <Dopant> E0.Percolation <value>
```

For the migration energy, the prefactor, the SiGe dependency, and the activation volumes for stresses, the specified material must be modeled as `full` or `simple` (in other words, any material that does not `discard` particles). For binding energies, only the `full` materials are valid. Percolation parameters are applied to `simple` and `full` materials.

Immobile species (substitutional dopants) have the migration prefactor set to 0, and the migration energy high, to clarify that the species will not perform diffusion steps. Finally, since Sentaurus Process KMC assumes substitutional atoms to be ionized (in other words,  $B^-$  and  $As^+$ ), the binding parameters (both the prefactor and the binding energy) are only defined for pairing reactions with a neutral  $I$  or  $V$ , such as  $B^- + I^0 \rightarrow B_i^-$  or  $As^+ + V^0 \rightarrow AsV^+$ . The binding energies for the other breakup reactions are computed automatically using these parameters.

## Parameter Examples

Silicon migration energies of boron particles:

```
sprocess> pdbGet Si KMC B Em
B    5.
BiM 0.5
Bi  0.25
BiP 1.1
```

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### Point Defects, Impurities, Dopants, and Impurity-Paired Point Defects

Prefactors of the above energies:

```
sprocess> pdbGet Si KMC B Dm  
B 0.  
BiM 1.e-3  
Bi 1.e-3  
BiP 1.e-3
```

Migration energies for boron in oxide (the only allowed boron particle is B):

```
sprocess> pdbGet Oxide KMC B Em  
B 3.53
```

Binding energy of boron in silicon:

```
sprocess> pdbGet Si KMC B Eb  
BiM 0.3
```

and prefactor:

```
sprocess> pdbGet Si KMC B Db  
BiM .37
```

Activation volumes for the formation energies of boron interstitial:

```
sprocess> pdbGet Si KMC B VF  
BiM -0.0044
```

Variation of formation energy with Ge concentration:

```
sprocess> pdbGet Si KMC B EfGe  
0
```

Finally, the binding energy cannot be defined for any material but full model ones, the result should be blank:

```
sprocess> pdbGet PolySilicon KMC B Eb
```

**NOTE** You can change these parameters whenever necessary to calibrate intrinsic and extrinsic dopant diffusivity under equilibrium conditions. For nonequilibrium conditions, you also can change the extended defects if necessary.

## Hopping Mode

To control the way Sentaurus Process KMC performs diffusion events, you can change the hopping mode using:

```
pbSet KMC HoppingMode <mode>
```

where `<mode>` can be `short`, `long`, `double`, or `longdouble` (default). Changing the hopping mode only changes the results statistically (that is, it is similar to changing the random seed); although, it may change the CPU time significantly.

### The short Mode

The `short` mode implies that the jumping distance for all the diffusion events  $\lambda$  is the same and equal to the second neighbor's distance. In addition, only one diffusion event is performed at a time.

### The long Mode

The `long` mode implies that the code increases the hopping distance to  $n\lambda$ , where  $n$  is an integer determined internally, in regions where there are no particles with which to interact. This increase improves the simulation performance in this area (in theory, by a factor of  $n^2$ ). In practice, the overall speed improvement is a factor of 2 or smaller, mainly because the empty regions where there are no particles to interact with are limited. The overhead is caused by the `long` mode implementation.

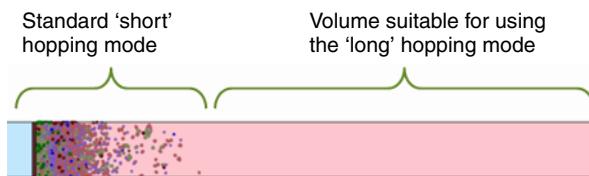


Figure 35 Even if the long hopping mode is available, it is used only for particles diffusing on empty volumes

### The double Mode

The `double` mode allows Sentaurus Process KMC to perform two diffusion events in one. Nevertheless, to properly account for interactions, the intermediate diffusion event is still simulated by Sentaurus Process KMC. Using this hopping mode saves 10% or less of CPU time.

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### The longdouble Mode

The `longdouble` mode is the fastest mode, and enables both long and double hops.

**NOTE** For more information on these hopping modes, refer to the literature [9].

---

## Enabling and Disabling Interactions

Interactions between particles are important. Whenever one mobile particle jumps into another particle, Sentaurus Process KMC tries to make both particles interact. These interactions may or may not be possible depending on whether the interaction is allowed and if it is energetically possible.

The interactions allowed between one mobile particle and other particles are specified in the parameter database using the parameter `ReactionsPointDefect`. The interactions between this type of defect are assumed to be always energetically favorable.

Consequently, changing the parameter `ReactionsPointDefect` is the only way to establish whether a moving particle will interact with other (mobile or immobile) particles. To change this parameter, use:

```
pdbSet <material> KMC <dopant> ReactionsPointDefect <string> <true | false>
```

This parameter needs a string and Boolean value. The Boolean value specifies if the interaction is allowed (`true`) or disallowed (`false`). The string contains the name of the two interacting particles, separated by a comma. For example:

```
sprocess> pdbGet Si KMC C ReactionsPointDefect
C,I      true
C,V      false
C,Ci    true
Ci,I    true
Ci,V    true
Ci,Ci   true
```

Therefore, in this example, the interaction between `C` and `V` is disabled. To enable it, use the command:

```
pdbSet Si KMC C ReactionsPointDefect C,V true
```

When enabling an interaction, the result does not have to be specified because Sentaurus Process KMC already knows it. The possible interaction results are:

PointDefect	Pairing reactions, in other words, dopants pairing with interstitials or vacancies to generate dopant–interstitial or dopant–vacancy particles. For example, B + I or As + IM.
AmorphousPocket	Reaction of interstitials or vacancies between them. For example, I + IM, I + V, or V + V. They involve both damage formation (mixed I and V) and small cluster creation (only I or V).
ImpurityCluster	Reactions involving the formation of impurity clusters, in other words, when the result has dopants and interstitials or vacancies with two or more of each. For example, Bi + I or AsV + AsV.

The reactions for each single charge state must be introduced, so the charged I also interacts with V and with other charge states of V:

```
sprocess> pdbGet Si KMC I ReactionsPointDefect
I,V      true
I,VM    true
I,VMM   true
I,VP    true
I,VPP   true
IP,V    true
IM,V    true
IM,IP   true
(...)
```

All interactions are listed in the parameter database. With that list of interactions, you can understand which reactions are considered and how they work.

## Interaction Rules

Sentaurus Process KMC does not accept all possible interactions within every two particles, but only interactions with a physical meaning, or with an available model. Consequently, the following rules apply:

- Reactions must include existing particles.
- Some reactions are only allowed in materials with full modeling.
- Reactions for a pair must be defined in the file of the involved dopant (for example, a reaction with Bi must be in the boron file, not in the interstitial file).
- If the result of a reaction does not exist, the reaction is discarded (that is, the reaction C + V is specified, but the particle CV is not defined).

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### Point Defects, Impurities, Dopants, and Impurity-Paired Point Defects

- Repulsive reactions are not allowed (for example,  $\text{Bi}^- + \text{Bi}^-$ ) except for ‘percolation’ models such as As + As or B + B (see [Percolation on page 475](#)).
- Reactions must satisfy microscopic reversibility. For example, if the reverse reaction is not possible, the reaction is discarded.
- Reactions creating impurity clusters must give a defined cluster. For example, Bi + Bi is allowed as long as there is a  $\text{B}_2\text{I}_2$  cluster defined; in this case, Bi + BiM would also be allowed.
- Only reactions producing defined `PointDefect`, `ImpurityCluster`, or `AmorphousPocket` are allowed. For example, Bi + C will generate an error message if there is no BCI cluster defined.

## Examples

**NOTE** Only advanced users should change the default interaction list because improper modifications can drastically change the diffusion models.

The interactions for boron are:

```
sprocess> pdbGet Si KMC B ReactionsPointDefect
B,I      true
Bi,I    true
Bi,V     true
BiM,V   true
BiP,V   true
B,Bi    false
B,BiP   true
B,IP    true
Bi,Bi   true
Bi,VM   true
Bi,VMM  true
Bi,VP   true
Bi,VPP  true
BiM,VP  true
BiM,VPP true
BiP,VM  true
BiP,VMM true
```

B and I can react, giving a mobile Bi particle. B and IP also give a Bi particle. The charge state of the resulting Bi particle is computed automatically by Sentaurus Process KMC depending on the Fermi level, temperature, and Bi levels in the band gap.  $\text{B}^- + \text{IM}$  is an electrostatically repulsive reaction, and is not allowed.

Bi possible charge states are neutral, positive, and negative. The reactions for these charge states should be specified as well. Bi and its different charges can react with I, V, and Bi. Bi + I produces an impurity cluster. Only microscopically reversible reactions are allowed. Because

a  $\text{Bi}_2$  cluster breaks up as  $\text{Bi} + \text{I}$ , any nonrepulsive reaction involving  $\text{Bi}$  and  $\text{I}$  is allowed.  $\text{Bi} + \text{V}$  recombines the IV pair, depositing substitutional boron. All nonrepulsive reactions between  $\text{B}_i$  and  $\text{V}$  are allowed, and all are specified in this example. Finally, there are more ways to produce impurity clusters including  $\text{BiP} + \text{B}$ , producing  $\text{B}_2\text{I}$ , and  $B_i^a + B_i^b \leftrightarrow \text{B}_2\text{I}_2$ , as long as  $a \cdot b \leq 0$  giving  $\text{B}_2\text{I}_2$ .

The reaction  $\text{B} + \text{V}$  is not specified here. Typing `B, V false` produces the same effect. Setting this reaction to `true` implies defining a  $\text{BV}$  particle (and its parameters) and specifying reactions for this  $\text{BV}$  particle, such as  $\text{BV} + \text{I} \rightarrow \text{B}$ .

## Defining Nonstandard Interactions

Sentaurus Process KMC allows you to define nonstandard interactions, which are intended to provide a mechanism for exceptional models that cannot be implemented using standard models and interactions. These reactions are of the type:



where  $\text{A}$ ,  $\text{B}$ , and  $\text{C}$  must be single particles (point defects or dopants). They are defined using `SpecialReaction` in the folder including the first species:

```
pdbSet Si KMC A SpecialReaction A,B,C true
```

The reactions defined with this mechanism are irreversible:  $\text{C}$  will not break into  $\text{A}$  and  $\text{B}$  back.

## Nonstandard Interaction Rules

The rules for nonstandard interactions are a subset of the rules for standard interactions (see [Interaction Rules on page 419](#)):

- Reactions must include existing particles. The result is always a point defect, not a cluster or another defect type.
- Reactions are only allowed in materials with `full` modeling.
- Reactions for a pair must be defined in the file of the involved dopant (for example, a reaction with  $\text{Bi}$  must be in the boron file, not in the interstitial file).
- If the result of a reaction does not exist, the reaction is discarded (that is, the reaction  $\text{C} + \text{V}$  is specified, but the particle  $\text{CV}$  is not defined).

In particular, these reactions can be nonconservative. For example, you can define a carbon-interstitial interaction giving arsenic ( $\text{C} + \text{I} \rightarrow \text{As}$ ). These reactions are nonstandard because they lack a physical sense, but they are allowed because they offer extra flexibility to define new models.

## 5: Atomistic Kinetic Monte Carlo Diffusion

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### Example

A model for nitrogen diffusion can be defined using a nonstandard interaction, in particular, when you want to model:



where  $N_{2,i}$  is mobile but  $N_2V$  is immobile. The second reaction is not a problem. You can define a dopant called  $Nn$  to be  $N_{2,i}$  and make it mobile, and you can define an  $NnV$  as the result of  $Nn + V$ . These reactions are standard.

The problem is that you cannot have an  $N + N$  reaction giving  $Nn$  using standard mechanisms. For this exception, you define  $N_i$  as  $N$  and use the special reaction:

```
pdbSet Si KMC N SpecialReaction N,N,Nn true
```

**NOTE** Special reactions are printed in the log file, for example:

```
KMC. Using special non-reversible reaction N + N -> Nn
```

---

## Stress Effects on Point Defects, Impurities, Dopants, and Impurity-Paired Point Defects

The stress model for Sentaurus Process KMC is disabled by default. To enable the stress model, use:

```
pdbSet KMC Stress 1
```

Alternatively, specify `kmc.stress` in the `diffuse` command:

```
diffuse kmc.stress time=...
```

Sentaurus Process KMC uses the stress provided by Sentaurus Process, but Sentaurus Process KMC does not compute it. The stress fields are updated from Sentaurus Process for each diffuse step.

Local stress dependency is introduced into Sentaurus Process KMC using the correction of the migration and binding energies of point defects and impurity-paired point defects.

Stress also affects the bandgap narrowing (see [Bandgap Narrowing on page 498](#)).

## Migration Energy

An anisotropic correction to the migration energy is introduced as:

$$\begin{bmatrix} \Delta E_m^x \\ \Delta E_m^y \\ \Delta E_m^z \end{bmatrix} = \begin{bmatrix} \Delta V_{par} & \Delta V_{ort} & \Delta V_{ort} \\ \Delta V_{ort} & \Delta V_{par} & \Delta V_{ort} \\ \Delta V_{ort} & \Delta V_{ort} & \Delta V_{par} \end{bmatrix} \begin{bmatrix} \sigma'_x \\ \sigma'_y \\ \sigma'_z \end{bmatrix} \quad (694)$$

where:

- $\Delta E_m^i$  are the corrections to the migration energy when diffusing in the  $i'$ -axis.
- $\sigma'_i$  are the principal stresses.
- $\Delta V_{par}$  and  $\Delta V_{ort}$  are the activation volumes for diffusion parallel and diffusion perpendicular to stress, respectively. They are included in the PDB as VD.

The relation between the  $i'$ -axes and the standard ones is established by a rotation  $R$  tensor, which diagonalizes the stresses tensor:

$$[R] \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{bmatrix} [R]^T = \begin{bmatrix} \sigma'_x & 0 & 0 \\ 0 & \sigma'_y & 0 \\ 0 & 0 & \sigma'_z \end{bmatrix} \quad (695)$$

The default setting of the parameter `ChangeAxis` is false (0), which disables this rotation, using the standard xyz axis instead of the  $i'$ -axes.

**NOTE** Setting `pdbSet KMC ChangeAxis 1` changes the direction of the hopping depending on the local stresses. This, in turn, dramatically impacts {311} dissolution because the structure is sensitive to the direction of the migrating incoming particles.

For more information, see [Interstitials and Vacancies on page 409](#).

## Binding Energy

The binding energy of an impurity-paired point defect  $A_i$  is corrected by:

$$\Delta E_b(A_i) = \frac{1}{3}(\sigma_{xx} + \sigma_{yy} + \sigma_{zz})(\Delta V_f(I) - \Delta V_f(A_i)) \quad (696)$$

where  $\Delta V_f$  is the activation volume for the formation energy. The activation energy for an impurity-paired point-defect breakup is defined (without stress) as the sum of the binding

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Point Defects, Impurities, Dopants, and Impurity-Paired Point Defects

energy and the migration energy of the emitted species ( $I$  for  $A_i$ ). Then, an extra correction of the migration energy of the emitted species under stress is needed.

Since the migration energy corrections depend on the axis, but the breakup of an impurity pair in Sentaurus Process KMC does not, an average of the corrections for all the axes is performed, and the frequency is computed as:

$$v^{stress}_{bk} = v^0_{bk} \exp(-\Delta E_b/(k_B T)) \frac{1}{3} \sum_i^{x,y,z} \exp(-\Delta E_m^i/(k_B T)) \quad (697)$$

where  $v^0_{bk}$  is the breakup frequency when there is no stress.

For more information, see [Impurities on page 411](#).

---

## Alloys

Alloys are included in Sentaurus Process KMC simulations as fields *not* as particles. Using Ge as an example of an alloy in Si, it means that Sentaurus Process KMC discards the particular position of Ge (the xyz coordinates) and only keeps track of how many Ge atoms were introduced in each internal element. This saves a huge amount of memory, while allowing Sentaurus Process KMC to account for SiGe effects. Ge diffusion is handled by solving a simple diffusion equation on the KMC elements. Because of this, there are some limitations:

- There are no Ge particles in the atomistic 3D plot.
- Ge (including implanted Ge) is shown as a field in the atomistic 3D plot.
- There are no events or reports associated with Ge because there are no Ge particles.
- There are no Ge models (for example, no Ge clusters) except for Ge diffusion.

This model can be used to:

- Simulate Ge diffusion.
- Include corrections to the migration and formation energies of point defects and impurity-paired defects when diffusing in SiGe materials.
- Include bandgap corrections due to SiGe.

**NOTE** Sentaurus Process KMC considers the effect of germanium whenever germanium is present. Continuum parameters (such as `Silicon`, `SiliconGermanium`, `ConversionConc`) do not affect Sentaurus Process KMC simulations.

## Alloy Diffusion

Ge will be used as an example of an alloy in Si material. Here, the Ge model diffusion implemented has been based partially on [10]. This model defines the diffusion of Ge in an indirect way through the use of  $\alpha$  of Is and Vs for a  $\text{Si}_{1-x}\text{Ge}_x$  material as:

$$\alpha_I = \frac{D_I^{Ge}(x)}{D_I^{Si}(x)} \quad (698)$$

where  $D_I^{Ge}(x)$  and  $D_I^{Si}(x)$  are the transport capacity associated with Ge and Si interstitials in  $\text{Si}_{1-x}\text{Ge}_x$ , respectively.

It can be assumed that these  $\alpha$ s follow the equation:

$$\alpha(x) = \alpha_{0,Si}^{1-x} \alpha_{0,Ge}^x \exp\left(-\frac{(1-x)E_{Si} + xE_{Ge}}{k_B T}\right) \quad (699)$$

where  $\alpha_{0,Si}$ ,  $\alpha_{0,Ge}$ ,  $E_{Si}$ , and  $E_{Ge}$  are input parameters specified in the PDB. Both interstitials and vacancies have a different  $\alpha$ .

**NOTE** The Ge diffusion model is switched on by default. To switch it off, set  $\alpha_{0,Si}$  and  $\alpha_{0,Ge}$  to null values.

**NOTE** For SiGe material, however, you must define the D0 and E parameters for the calculation of  $\alpha$  in Si and Ge. By default, it will take the values defined in Si and Ge as D0alphaSi, EalphaSi, Alloy.D0alpha, Alloy.Ealpha, and so on.

## Parameters

The parameters  $\alpha_{0,Si}$ ,  $\alpha_{0,Ge}$ ,  $E_{Si}$ , and  $E_{Ge}$  are specified in the PDB with the names D0alphaSi, Alloy.D0alpha, EalphaSi, and Alloy.Ealpha. In particular:

```
sprocess> pdbGet Si KMC I EalphaSi
0.4
sprocess> pdbGet Si KMC I Alloy.Ealpha
0
sprocess> pdbGet Si KMC I D0alphaSi
35
sprocess> pdbGet Si KMC I D0alphaGe
2.2
sprocess> pdbGet Si KMC V EalphaSi
0.25
sprocess> pdbGet Si KMC V EalphaGe
0
```

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```
sprocess> pdbGet Si KMC V D0alphaSi  
30  
sprocess> pdbGet Si KMC V D0alphaGe  
2.2
```

## Alloy Effects

The following sections discuss alloy effects on point defects, impurities, dopants, and impurity-paired point defects. In the next sections, Ge in silicon is used as an example for these models.

### Migration and Formation Energies

The corrections  $\Delta E_m = \alpha_m[\text{Ge}]$  and  $\Delta E_f = \alpha_f[\text{Ge}]$  are added to the migration and the formation energies, respectively.  $[\text{Ge}]$  is the germanium concentration, and  $\alpha_m, \alpha_f$  are the dependencies of energies with Ge concentration for migration and formation.

### Binding Energy

The binding energy of an impurity-paired point defect  $A_i$  is corrected by:

$$\Delta E_b(A_i) = [\text{Ge}](\alpha_f(I) + \alpha_f(A) - \alpha_f(A_i)) \quad (700)$$

For more information, see [Impurities on page 411](#).

### Bandgap Narrowing

The Ge inclusion changes the band gap as explained in [Bandgap Narrowing on page 498](#).

### Parameter Interpolation in Alloys

You can interpolate relevant parameters from the base materials. For example, parameters in SiGe will be interpolated from their respective values in Silicon and Germanium. Most Double and DoubleArray type parameters are interpolated, but other types of parameter such as Switch, String, and Boolean, as well as some Double and DoubleArray, are not interpolated.

Because SiGe is by default *like* Silicon, parameters that are not interpolated will be the same as in Silicon. For details about parameter inheritance using like materials, see [Like Materials: Material Parameter Inheritance on page 24](#).

In addition, if a parameter is specified directly in the alloy (for example, directly in SiGe), the value is used as specified and is not interpolated.

The set of parameters that are interpolated can be printed to the log file using the command:

```
print_interpolated_params [Diffuse | KMC | Mechanics]
```

This command must be called after the expected parameter interpolation has occurred (see [print\\_interpolated\\_params on page 1136](#)).

Parameter interpolation is switched on by default in SiGe and switched off by default in Silicon and Germanium.

**NOTE** For example, in Ge-doped silicon, parameter interpolation is switched off by default for backward compatibility and default silicon behavior should be expected. Parameter interpolation can be switched on in this case by setting:

```
pdbSet Si Skip.Parameter.Interpolation 0
```

Similar to other Sentaurus Process modules, parameter interpolation in Sentaurus Process KMC allows linear, piecewise linear, parabolic, and logarithmic interpolation. For piecewise linear interpolation, a table with parameter values for different mole fractions must be provided. For parabolic interpolation, a parameter with the .x2 suffix must be defined.

For details about parameter interpolation, see [Alloy Materials and Parameter Interpolation on page 25](#).

## Alloy Condensation at Growing Interface

You can simulate alloy condensation or pileup at interfaces. The physical mechanism implemented is similar to snow plowing dopants during silicidation. The parameters Pref.GrowthDeposit and Ener.GrowthDeposit allow you to control the redistribution of alloys from growing oxide to substrate. The probability of alloy transfer to oxide is calculated using the following Arrhenius expression:

$$p = \text{Pref.GrowthDeposit} \times \exp\left(-\frac{\text{Ener.GrowthDeposit}}{kT}\right) \quad (701)$$

Allowed values of Pref.GrowthDeposit are between 0 and 1. The default is 1, which means the alloy will stay in the growing oxide side. The default value of Ener.GrowthDeposit is 0. These parameters can be obtained as follows:

```
sprocess> pdbGet Oxide_Silicon KMC Ge Pref.GrowthDeposit
1.0

sprocess> pdbGet Oxide_Silicon KMC Ge Ener.GrowthDeposit
0.0
```

## Introducing Alloys in Simulations

Alloys can be introduced into simulations by:

- Using implantation.
- Using the `select` command.
- Atomizing a previous continuum structure with the alloy.
- Using `kmc add` to explicitly add it.
- Depositing a layer doped with the alloy.

---

## Damage Accumulation Model: Amorphous Pockets

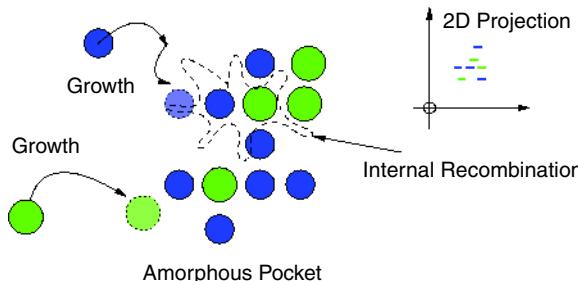
Damage accumulation evolution, that is, the evolution of small interstitial and vacancy clusters after ion implantations, is a crucial step that affects the subsequent formation of extended defects and impurity clusters. This accumulation generates the TED of commonly used dopants, such as boron.

Experimentally, electron irradiation and light-ion implantation create isolated point defects inside the silicon. In contrast, heavy ions generate highly disordered regions called *amorphous pockets* (APs) as a consequence of the implanted cascades. Depending strongly on the temperature, ion mass, and dose rate, this disordered region can dissolve as a result of internal recombination or can grow until an amorphous layer is created. The activation energy for annealing this damage varies in the literature, 0.9 eV [11] at room temperature, 1.2 eV for 400°C to 550°C, but it is much less than the 2.7 eV reported for truly amorphized amorphous layers. This means the damage accumulation depends on the dynamic annealing, ripening, and dissolution history of the APs during the implantation process. This annealing can have a quasi-continuum range of activation energies.

There is much discussion on how this damage is annealed. Some papers point to an annealing of the disordered region [12]: APs using an internal recombination of *IV* pairs rather than through the emission of point defects. Only when the AP does not contain further *IV* pairs does it begin to emit its remaining *I*s or *V*s, behaving as a small *I* or *V* cluster.

Sentaurus Process KMC simulates the damage accumulation using APs, disordered collections of point defects (*I*s and *V*s) stable at low temperatures. APs dissolve fast at higher temperatures, leaving only clusters with the net excess of *I*s or *V*s. APs can contain *IV* pairs or only *I*s and *V*s. In the first case, APs try to recombine the pairs; in the second case, APs behave as small clusters and can emit their constituent particles. Whenever an AP containing only *I*s or *V*s (but not *IV* pairs) reaches a threshold size, the AP transforms into an extended defect ({311}s and loops for *I*s, voids for *V*s).

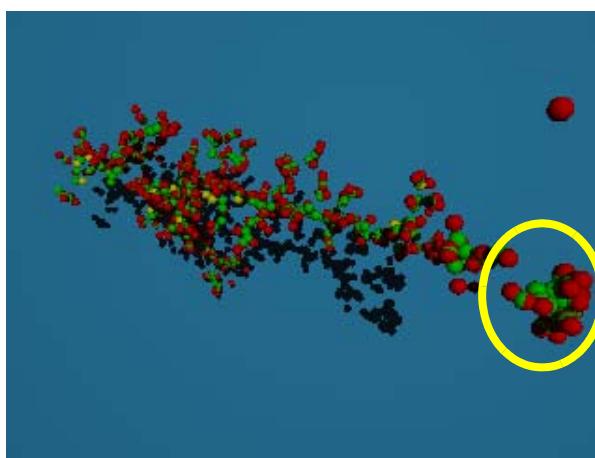
APs can grow capturing new incoming point defects, and they can dissolve by internal recombination of *IV* pairs or by particle emission when there are no more *IV* pairs (see [Figure 36](#)).



[Figure 36](#) Growth of APs showing their internal recombination

## Shape of Amorphous Pockets

APs have an irregular shape. Sentaurus Process KMC does not reshape the defect as new; incoming particles join the AP: particles are left in their incoming positions. [Figure 37](#) shows some APs resulting from an implanted cascade.



[Figure 37](#) APs formed in Sentaurus Process KMC after some implanted as cascades: interstitials are red, vacancies are green, arsenic is yellow

## Growth of Amorphous Pockets

APs capture any incoming point defect (*I* or *V*) within their capture radius. The capture radius of APs is the sum of all their constituent particles. Point defects with any charge state are captured by APs containing both *Is* and *Vs*. Only neutral *Is* or *Vs* are captured when APs contain only *Is* or only *Vs*.

## Recombination

APs containing  $IV$  pairs (that is, APs with both interstitials and vacancies) can recombine pairs using a recombination event, which recombines one  $I$  with one  $V$  at a time. This event is performed with a frequency given by:

$$v_{diss} = v_{0, diss} \cdot \text{size}^\beta \exp(-(E_{diss}(\text{size}) + P\Delta V_{diss} + \alpha_{IV}[Ge])/(k_B T)) \quad (702)$$

where:

- The prefactor  $v_{0, diss}$  is called `D0.AmorphousPocket` in the parameter database.
- `size` is the size of the cluster.

The size of a cluster  $I_n V_m$  is a Tcl procedure of `n` and `m` specified in the file `KMC.tcl` under the name `getAmorphousPocketSize` (the procedure can be modified):

```
fproc getAmorphousPocketSize { sizeI sizeV } {
    return [expr ($sizeI + $sizeV)/2]
}
```

- $\beta$  is an exponent called `Exponent.AmorphousPocket`.
- $E_{diss}$  depends on the size of the AP and is specified as a list of energies for each size (`Eb.AmorphousPocket`). The different sizes are specified as `IxeVx`. If an energy is not specified for a size, Sentaurus Process KMC takes the linear interpolation between the last two specified values. For sizes higher than the last specified size, the last specified energy is assigned automatically.
- $\alpha_{IV}$  is the germanium correction to recombination (`Alloy.Eb.AmorphousPocket`).
- $P$  is the hydrostatic pressure.
- $\Delta V_{diss}$  is the activation volume for the AP dissolution (`VF.AmorphousPocket`).

## Parameters

The parameters needed by the damage accumulation model are specified using:

```
pdbSet Si KMC Damage <Parameter> <value>
```

For example:

```
sprocess> pdbGet Si KMC Damage D0.AmorphousPocket
0.0005
sprocess> pdbGet Si KMC Damage Exponent.AmorphousPocket
0.66
sprocess> pdbGet Si KMC Damage VF.AmorphousPocket
0
```

```
sprocess> pdbGet Si KMC Damage Eb.AmorphousPocket
IV          0.65
I199V199    2.4
sprocess> pdbGet Si KMC Damage Alloy.Eb.AmorphousPocket
0
```

For the above parameters, the `Eb.AmorphousPocket` values for  $I_x V_x$ , with  $x > 1$  and  $x < 199$  will be generated by Sentaurus Process KMC as a linear interpolation between the points (1, 0.65) and (199, 2.4):

```
Silicon/Damage Eb.AmorphousPocket (IV) = 0.65
Silicon/Damage Eb.AmorphousPocket Interpolated (2) = 0.658838
Silicon/Damage Eb.AmorphousPocket Interpolated (3) = 0.667677
...

```

**NOTE** You can change these parameters to calibrate the damage accumulation model.

**NOTE** The maximum size allowed for IV clusters is  $I_{249} V_{249}$ .

## Emission

When all *IV* pairs have been recombined, APs behave as small *I* or *V* clusters, allowing the emission of their extra constituent particles. These defects emit neutral *Is* or *Vs* particles with a frequency given by:

$$v_{emit} = v_{0,emit} \cdot \exp(-E_{emit}(size)/(k_B T)) \quad (703)$$

The prefactor is proportional to the input parameter `D0.Cluster`, but also includes a dependency on the size of the cluster. The activation energy for emission of an *X* (either *I* or *V*) is:

$$E_{emit} = E_b(X) + E_m(X) + \Delta E_b(X) + \Delta E_m(X) \quad (704)$$

the sum of the corrected binding energy (that depends on the cluster size) and the migration energy. The cluster size is defined as the number of contained *Is* or *Vs* (see [Figure 38](#) on [page 432](#)).

## 5: Atomistic Kinetic Monte Carlo Diffusion

Damage Accumulation Model: Amorphous Pockets

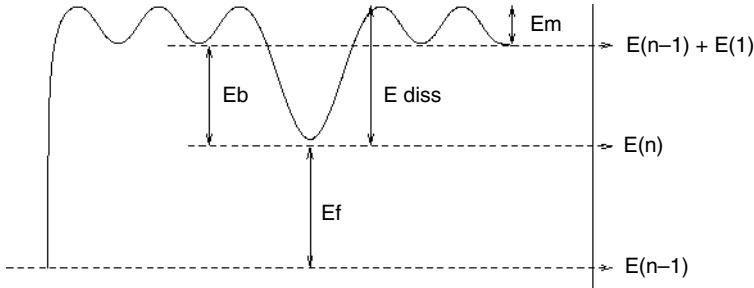


Figure 38 Energies involved in emission of an  $n$ -sized cluster

The parameter D0.Cluster is the constant proportional to the emission prefactor, and Eb.Cluster is the cluster binding energy, where dependency with size is explicitly assigned. For sizes bigger than the last specified cluster, the binding energies are computed using:

$$E_b(\text{size}) = E_{b,L} - (E_{b,L} - E_{b,S}) \frac{\text{size}^a - (\text{size} - 1)^a}{2^a - 1} \quad (705)$$

where:

- $E_{b,L}$  (Eb.LargeCluster) is the binding energy for the largest cluster.
- $E_{b,S}$  (Eb.SmallestCluster) is the binding energy for the smallest cluster (size 1).
- $a$  (Exponent.Cluster) is the exponent, usually 2/3 or 3/4.

Figure 39 shows some binding energy values and compares them with the numbers obtained using Eq. 705.

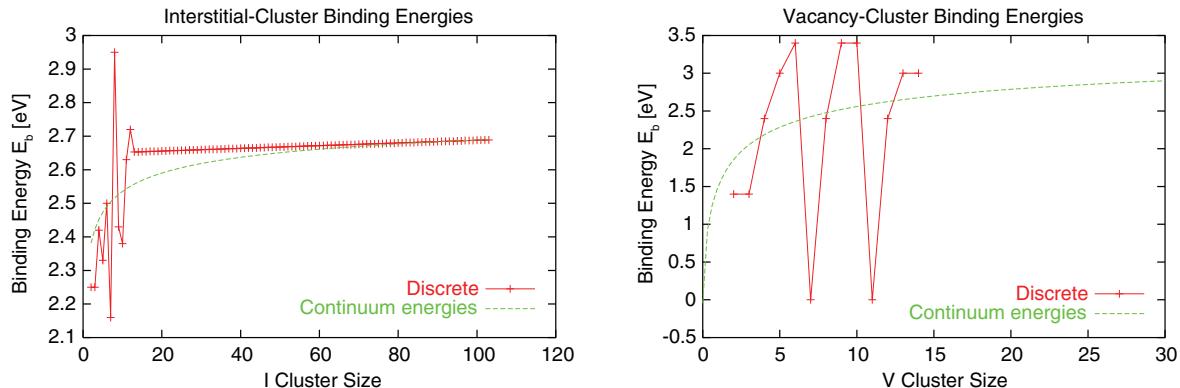


Figure 39 (Left) Interstitial-cluster binding energies and (right) vacancy-cluster binding energies; discrete values are assigned in the parameter database and the continuum energies are computed using Eq. 705

Finally, the correction applied for the migration is the normal one:

$$\Delta E_m(X) = \alpha_m[Ge] + \frac{1}{3} \sum_i^{x,y,z} \exp(-\Delta E_m^i/(k_B T)) \quad (706)$$

and for the binding of the particle to the cluster is:

$$\Delta E_b(X) = P \Delta V_b^{extended}(X) + \alpha_{Cl}[Ge] \quad (707)$$

where  $\Delta V_b^{extended}$  is called VF.Cluster in the PDB, and  $\alpha_{Cl}$  is the germanium correction to binding (Alloy.Eb.Cluster).

## Parameters

The parameters for *Is* and *Vs* emission are specified only for the silicon material. They can be found in the interstitial and vacancy files included in the parameter database.

### Prefactors

```
sprocess> pdbGet Si KMC I D0.Cluster
150.0
sprocess> pdbGet Si KMC V D0.Cluster
10
```

### Energies

```
sprocess> pdbGet Si KMC I Eb.Cluster
I2      2.45
I3      2.45
(...)
I13     2.853
I103    2.889

sprocess> pdbGet Si KMC V Eb.Cluster
V2      1.4
V3      1.4
V4      2.4
(...)
```

For sizes between specified sizes (for example, I14 to I102), the parameters are computed as linear interpolations of the specified values:

```
Silicon/I Eb.Cluster(I13) = 2.853
Silicon/I Eb.Cluster Interpolated (14) = 2.8534
(...)
Silicon/I Eb.Cluster Interpolated (102) = 2.8886
Silicon/I Eb.Cluster(I103) = 2.889
```

and parameters for [Eq. 704, p. 431](#):

```
sprocess> pdbGet Si KMC I Eb.SmallestCluster  
2.51  
sprocess> pdbGet Si KMC I Eb.LargeCluster  
3.09  
sprocess> pdbGet Si KMC I Exponent.Cluster  
0.75  
sprocess> pdbGet Si KMC V Eb.SmallestCluster  
1.5  
sprocess> pdbGet Si KMC V Eb.LargeCluster  
3.7  
sprocess> pdbGet Si KMC V Exponent.Cluster  
0.6667
```

**NOTE** When changing these parameters, their values affect not only the damage accumulation model, but also the interstitial and vacancy supersaturation and, consequently, the TED. Because the damage accumulation model is the seed for subsequent extended defects or recrystallization, these values also affect the formation of extended defects.

---

## Amorphous Pockets Life Cycle

Whenever two point defects ( $I + I$ ,  $V + V$ , or  $I + V$ ) interact with each other, an AP is generated. When the AP is formed, subsequent incoming  $I_s$  or  $V_s$  are captured and added to the AP. If the AP contains at least one  $IV$  pair, the AP recombines the  $IV$  pairs. The  $IV$  pair frequency depends on the number of  $IV$  pairs present in the AP. If there are only  $I_s$  or  $V_s$  in the AP, the AP emits  $I_s$  or  $V_s$ .

The evolution of APs can follow three paths:

- APs can dissolve recombining internal  $IV$  pairs, emitting point defects, or both.
- AP containing only  $I_s$  or  $V_s$  may be transformed into extended defects: {311} defects and dislocation loops for  $I_s$  and voids for  $V_s$ .
- If the concentration of some of the boxes (the internal Sentaurus Process KMC grid elements) containing the AP reaches a concentration threshold, the element is considered amorphous and its particles are removed from the AP. Consequently, APs only exist in crystalline silicon.

For example, assuming there is an AP with two  $V_s$  and seven  $I_s$  ( $I_7V_2$ ), since the AP contains both  $I_s$  and  $V_s$ , the only possible event is the recombination of  $IV$  pairs. The first  $IV$  pair recombines with the recombination energy assigned to size 2, leaving an  $I_6V_1$ . The second recombination energy, with a recombination energy assigned to size 1, leaves an  $I_5$  AP. This

AP begins to emit *I*s, with a frequency associated to its size (5). However, if it captures a *V*, it becomes an  $I_5V_1$  and must recombine the *IV* pair with an associated recombination size of 1.

An AP must satisfy the following conditions before being transformed into a {311} defect or void:

- It can contain only *I*s or only *V*s, but not both.
- It must be bigger than or equal to a threshold size.
- Transition must be enabled.

The threshold size is specified with the parameters `Min.311.Size` and `Min.111Loop.Size` for *I*s, and `Min.Void.Size` for *V*s. The transition is enabled by a value between 0 and 1. This value is computed as:

$$P = E_0 \times \exp((-E + \Delta E)/(k_B T)) \quad (708)$$

The prefactor  $E_0$  is specified as `D0.AP.To.311` for {311}s, `D0.AP.To.111Loop` for {111} loops, and `D.AP.To.Void` for voids, and the energies are specified as `E.AP.To.311`, `E.AP.To.111Loop`, and `E.AP.To.Void`. For {311}s,  $\Delta E$  are the corrections for pressure and Ge. For voids,  $\Delta E = 0$ :

$$\Delta E = PV_{311toLoop} + \alpha_{311toLoop}[Ge] \quad (709)$$

The volume correction is called `vF.311.To.Loop`, and the germanium correction is called `Alloy.E.311.To.Loop`.

For  $P = 0$ , the transition is disabled. For  $P = 1$ , it is enabled. For  $P > 1$ , the value is rounded to 1. Values between 0 and 1 establish a probability for the transition.

## Parameters

Minimum sizes for the transitions:

```
sprocess> pdbGet Si KMC I Min.311.Size
33
sprocess> pdbGet Si KMC I Min.111Loop.Size
33
sprocess> pdbGet Si KMC V Min.Void.Size
27
```

Transition probabilities:

```
sprocess> pdbGet Si KMC Damage D0.AP.To.311
200000000.0
sprocess> pdbGet Si KMC Damage E.AP.To.311
1.3
```

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Damage Accumulation Model: Amorphous Pockets

```
sprocess> pdbGet Si KMC Damage D0.AP.To.111Loop  
100000000.0  
sprocess> pdbGet Si KMC Damage E.AP.To.111Loop  
1.3  
sprocess> pdbGet Si KMC Damage D0.AP.To.Void  
200000000.0  
sprocess> pdbGet Si KMC Damage E.AP.To.Void  
1.3
```

---

## Interactions of Amorphous Pockets

To change the default AP interactions, use the parameters `ReactionsClusterI`, `ReactionsClusterV`, and `ReactionsClusterIV`. These parameters control the reactions between APs containing only interstitials, only vacancies, or both. APs can react not only with *I*s and *V*s, but also with dopants. In this latter case, the result of the reaction must be specified.

### Interaction With Point Defects: I and V

To customize AP reactions, change the parameters defined for *I*, *V*, and *IV* clusters using the command:

```
pdbSet Si KMC Damage <ReactionsClusterType> <species> <true | false>
```

For example, the following command disables the reaction  $I_n + I \rightarrow I_{n+1}$  for small clusters:

```
pdbSet Si KMC Damage ReactionsClusterI I false
```

Consequently, it disables the ripening of these clusters. The following command disables the recombination of *I* with small vacancy clusters:

```
pdbSet Si KMC Damage ReactionsClusterV I false
```

### Parameters

Small interstitial and vacancy clusters may react with neutral interstitials and vacancies. Charged interstitials or vacancies are not allowed due to microscopic reversibility reasons:

```
sprocess> pdbGet Si KMC Damage ReactionsClusterI  
          I      true  
          V      true  
sprocess> pdbGet Si KMC Damage ReactionsClusterV  
          I      true  
          V      true
```

APs with both *I*s and *V*s accept interstitials or vacancies with any charge. In this case, because they do not emit particles, there are no microscopic reversibility restrictions:

```
sprocess> pdbGet Si KMC Damage ReactionsClusterIV
          I      true
          IP     true
          IM     true
          V      true
          VP     true
          VPP    true
          VM     true
          VMM    true
```

## Interaction With Impurities

APs do not trap impurities but can interact with them. In this interaction, impurities can lose a point defect, becoming substitutional (for example,  $B_i + I_2V_3 \rightarrow B + I_3V_3$ ) or can gain some of them being transformed into an impurity cluster (for example,  $B_i + I_2V_3 \rightarrow BI_2 + IV_3$ ). Consequently, the interaction within impurities and APs plays a crucial role in deactivating dopants, typically during implantation and low-temperature annealings.

To control these interactions, use:

```
pdbSet Si KMC <impurity> <ReactionsClusterType> <species,result>
          <true | false>
```

`ReactionsClusterType` can be `ReactionsClusterI` for small *I* clusters, `ReactionsClusterV` for small *V* clusters, and `ReactionsClusterIV` for mixed clusters.

For example, the reaction  $B_i^- + I_nV_m \rightarrow BI_2 + I_{n-1}V_m$  can be disabled for mixed clusters with:

```
pdbSet Si KMC B ReactionsClusterIV BiM,BI2 false
```

**NOTE** A comma must separate the incoming particle from the result, without any space in between.

## Parameters

The reactions between boron (for example) and mixed clusters can be displayed with:

```
sprocess> pdbGet Si KMC B ReactionsClusterIV
          BiM,BI2 true
          Bi,BI2 true
          BiP,BI2 true
          B,BI2   true
```

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Extended Defects

There are no reactions between boron and vacancy clusters:

```
sprocess> pdbGet Si KMC B ReactionsClusterV
```

The reactions between boron and small  $I$  clusters are disabled:

```
sprocess> pdbGet Si KMC B ReactionsClusterI
Bi,BI2  false
BiM,BI2 false
```

---

## Extended Defects

Small clusters are defined as immobile agglomerations of interstitials or vacancies, and are modeled using AP defects. When the number of  $I_s$  or  $V_s$  in these clusters grows above a specified threshold, the small clusters are converted into extended defects ( $\{311\}$  or void type). Finally, when the ripening of  $\{311\}$ s overcomes some limit, the  $\{311\}$ s are transformed into dislocation loops.

---

## $\{311\}$ Defects (ThreeOneOne)

The  $\{311\}$  *rod-like* defects are associated with TED [13]. Consequently, they need a realistic simulation, in both shape and energetic values. Its shape is like rectangular stripes of interstitials lying on a  $\{311\}$  plane along a  $<110>$  direction. Takeda [14] gives an atomic model for its structure, whose stability has been confirmed by theoretical studies [15][16][17].

### Shape of $\{311\}$ Defects

Sentaurus Process KMC models  $\{311\}$  defects as parallel stripes (rows) of  $I$  particles lying in one of the twelve orientations, randomly chosen, of a  $\{311\}$  plane. The  $\{311\}$  shape is modeled as  $N_r$  rows of  $I_s$  lying on a  $<01\bar{1}>$  line with a distance of  $a/\sqrt{2}$  between  $I_s$  in the same line, and as  $N_c$  columns keeping a distance of  $a\sqrt{2}/4$  between them, with  $a = 0.543$  nm, the silicon lattice constant.

The ratio between the length ( $L$ ) and the width ( $W$ ) is given by:

$$W \approx \sqrt{CL} \quad (710)$$

where  $C = 0.5$  nm. This ratio is maintained, reshaping the  $\{311\}$  defect (that is, changing the number of row and columns) when necessary (see [Figure 40 on page 439](#)).

The  $\{311\}$  defects only exist above a size threshold. Smaller defects are assumed to be APs, and they have an irregular shape (see [Amorphous Pockets Life Cycle on page 434](#)).

When {311} defects grow enough, they are transformed into dislocation loops (see [Dislocation Loops on page 442](#)). The threshold size (number of interstitials) between {311} defects and dislocation loops is assumed to follow an Arrhenius plot:

$$\text{size} = \text{prefactor} \times \exp(E/(k_B T)) \quad (711)$$

The formation energy of the dislocation loop must be smaller than the {311} formation energy at the threshold size; otherwise, the threshold is taken as the size where both energies are equal.

Both prefactor and E are parameters available in the parameter database with the names D0.311.To.Loop and E.311.To.Loop, respectively.

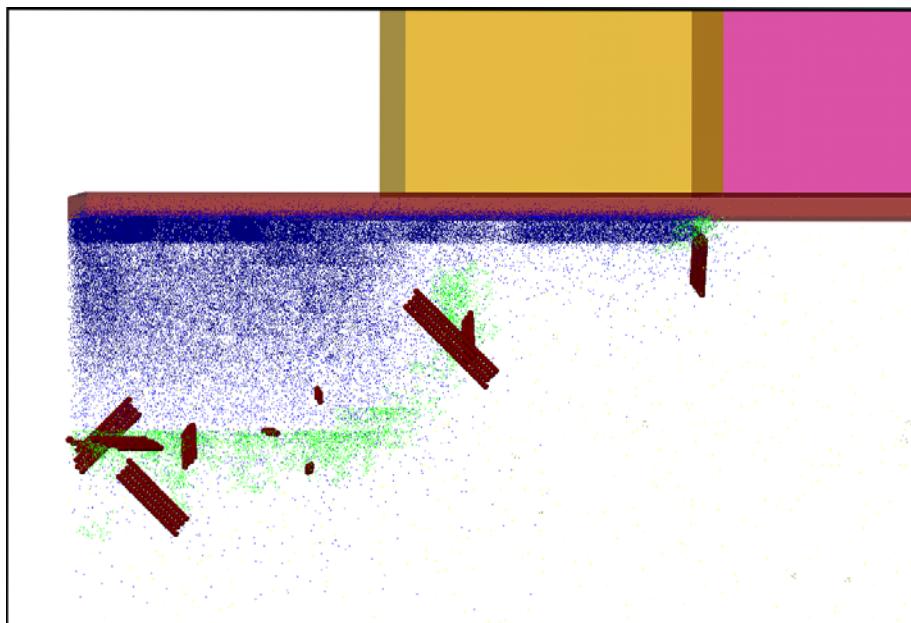


Figure 40 {311} defects are simulated as parallel stripes (rows) of I particles lying in a {311} plane: red is silicon interstitials in {311}; green is I and V in APs; and blue is arsenic

## Parameters

The parameters to control the transformation between {311} defects and dislocation loops are specified for interstitials in silicon:

```
sprocess> pdbGet Si KMC I D0.311.To.Loop
1.6
sprocess> pdbGet Si KMC I E.311.To.Loop
0.68
```

**NOTE** These parameters can be changed to fit the {311} defect to a dislocation loop transition size.

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Extended Defects

## Capture

Each time a neutral  $I$  point defect interacts with an  $I$  belonging to a  $\{311\}$  defect, the  $\{311\}$  captures the point defect. Since  $\{311\}$  defects grow and shrink at their ends, the new particle is attached at the nearest end of the defect. When the end cannot grow because it is too close to an interface or a boundary, the other end is used.

When `311.Dopant.Model 1` is set, impurities also can be trapped. These trapped impurities will remain in the captured location until they are re-emitted. Only neutral impurities (or neutral impurity pairs) are captured and re-emitted.

## Emission

To preserve microscopic reversibility between the capture and the emission processes, emitted particles (neutral interstitials) are taken randomly from one of the two ends and released from a random point at the  $\{311\}$  surface (see [Figure 41](#)).

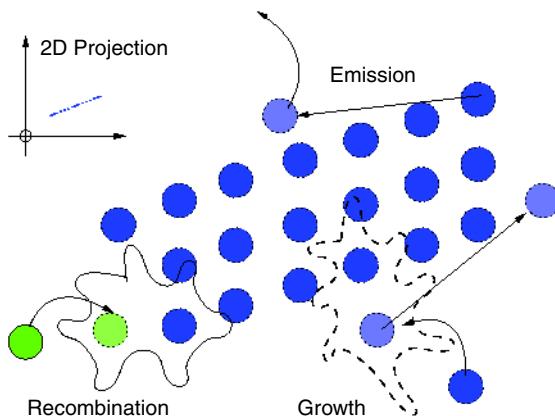


Figure 41 Recombination of defects in a  $\{311\}$  defect

The emission frequency is computed as in APs by:

$$v_{emit} = v_{0,emit} \times \exp((-E_{emit}(size) + P\Delta V_{311} + \alpha_{311}[Ge])/(k_B T)) \quad (712)$$

where the considerations for the AP emission, including all the corrections, apply. The binding energies are taken from the list supplied with the `Eb.Cluster` parameter. These energies are shared with the APs. As previously explained, for sizes less than a threshold value, defects are considered APs. Otherwise, they are rearranged as  $\{311\}$  defects. Consequently, only binding energies for sizes equal to or greater than the AP- $\{311\}$  threshold apply to  $\{311\}$  defects. Corrections are applied for both pressure and germanium content. These corrections are specified as `VF.311` and `Alloy.Eb.311`, respectively.

In addition, {311} defects may emit captured dopants if `311.Dopant.Model` 1 is set. The emission frequency for them is:

$$v_{emit}(A_i) = v_{0, emit}(A_i) \times \exp(-E_{emit}((A_i)/(k_B T))) \quad (713)$$

The prefactor and the activation energy are called `D0.311` and `Eb.311`, respectively, in the PDB.

## Parameters

For impurity re-emission, the parameters are:

```
sprocess> pdbGet Si KMC In D0.311
200.0
sprocess> pdbGet Si KMC In Eb.311
2.0
```

## Recombination

The {311} defects recombine incoming Vs with any charge by annihilating the *I*s at the nearest {311} defect end. When {311} defects dissolve, they do not become APs when the AP-{311} threshold size is reached. The emission frequency depends on the binding energy, and the binding energy only depends on the size of the defect. Since a interstitial cluster and a small {311} defect have the same binding energy when they have the same size, the defect shape affects only the capture volume, but not the emission frequency. Consequently, rearranging {311} defects as small defects, and vice versa, only changes the capture volume, and these changes are negligible for small clusters. Nevertheless, the capture volume differences between small {311} defects and irregular clusters are negligible, and there is no information about the shape of dissolving {311} defects.

Finally, when a {311} defect reaches size 2, it releases the particles as two interstitials and the {311} defect disappears.

## Interactions

Interactions between {311} defects and mobile particles can be modified with:

```
pdbSet Si KMC <I | V | Impurities> Reactions311 <species> <true | false>
```

Growth reactions ( $I_n + I$ ) are controlled with *I*, and recombination reactions ( $I_n + V$ ) with *V*. {311} defects can break up paired dopants capturing the interstitial or recombining the vacancy (for example,  $B_i + I_n \rightarrow B + I_{n+1}$ ). The remaining dopant will be immediately released or captured (and re-emitted later) by the defect depending on the value of the parameter `311.Dopant.Model` (0 releases dopants, 1 traps it). A captured dopant can be re-emitted. These reactions enable the {311} to decrease the impurity diffusion.

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Extended Defects

Only neutral  $I_S$  react with  $\{311\}$  defects and, consequently, only paired dopants with the same charge as the substitutional dopant react with  $\{311\}$  defects. Any charge state is allowed for the recombination of vacancies.

### Parameters

Use the following for growth and recombination:

```
sprocess> pdbGet Si KMC I Reactions311
I      true
sprocess> pdbGet Si KMC V Reactions311
V      true
```

For paired impurity breakup (boron, for example), use:

```
sprocess> pdbGet Si KMC B Reactions311
BIM    false
sprocess> pdbGet Si KMC I 311.Dopant.Model
0
```

You can define the parameter `311.Dopant.Model` globally as a default for all dopants, but define it locally with a different value that overwrites the global value for a particular dopant. For example, the following commands set the model for all the impurities as ‘release dopant,’ except for boron:

```
pdbSet Si KMC I 311.Dopant.Model 0
pdbSetDouble Si KMC B 311.Dopant.Model 1
```

---

## Dislocation Loops

Dislocation loops are planar defects lying on  $\{111\}$  planes [18]. A dislocation loop can be either a faulted dislocation loop (FDL) or perfect dislocation loop (PDL). FDLs are circular stacking faults surrounded by a dislocation line. PDLs are not implemented in Sentaurus Process KMC.

The  $\{311\}$  defects are precursors of dislocation loops. When the implantation conditions (available concentration of  $I$ , distance to the free surface) are appropriate,  $\{311\}$  defects grow until they reach the threshold size and transform into dislocation loops. Dislocation loops are more stable than  $\{311\}$  defects; consequently, the supersaturation created by dislocation loops is lower.

## Shape of Dislocation Loops

The shape of dislocation loops is computed as a filled circle in a {111} orientation (see [Figure 42](#)). All {111} orientations are allowed, and one is randomly chosen.

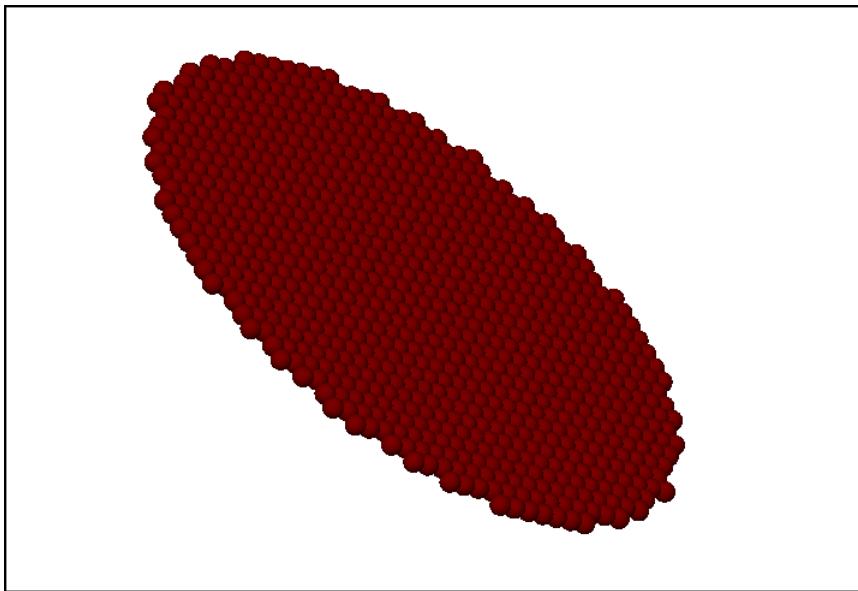


Figure 42 A dislocation loop taken from a Sentaurus Process KMC simulation

## Capture

Dislocation loops capture any incoming neutral interstitial. The original position is lost, and the particle is moved to the proper position in the disk. The capture radius is the sum of the capture radius of the constituent particles.

When the `ReactionsLoop` is set and `Loop.Dopant.Model` is `true`, dislocation loops capture incoming impurities. When `Loop.Dopant.Model` is `false`, the impurity is not captured. However, when it carries a point defect (in other words, is an impurity pair), the pair is broken; the impurity is deposited as a substitutional impurity; and the point defect reacts with the loop.

## Emission

Dislocation loops emit neutral interstitials with a frequency given by:

$$v_{emiss} = v_{0, emiss} \times \exp\left(-\frac{E_{b, loop}(size) + E_m(I) + \Delta E_m(I) + \Delta E_{b, loop}}{k_B T}\right) \quad (714)$$

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Extended Defects

where:

- $v_{0, emiss}$  includes both a prefactor and a linear dependency on the dislocation loop size.
- $E_{b, loop}(\text{size})$  is the binding energy of the dislocation loop, which only depends on the size.

Sentaurus Process KMC computes the binding energies as:

$$E_{b, loop}(\text{size}) = E_f(I) + E_{f, loop}(\text{size} - 1) - E_{f, loop}(\text{size}) \quad (715)$$

The dislocation loop formation energies are taken from [19] as:

$$E_{f, loop}(\text{size}) = \pi\gamma R^2 + \frac{a^2\mu}{6(1-\nu)} \cdot R \cdot \log\left(\frac{8R}{b}\right) - nE_f(I) \quad (716)$$

where:

- $R = \sqrt{\text{size}/(\pi d_{111})}$  is the loop radius.
- $\gamma$  is the stacking fault energy per unit area.
- $\mu$  is the shear modulus.
- $\nu$  is the Poisson ratio.
- $b$  is the Burgers vector modulus.
- $a$  is the silicon lattice parameter.
- $d_{111}$  is the atomic density in a {111} plane, in nm<sup>-2</sup>.

The above parameters are specified in the parameter database:  $\gamma$  is called gamma,  $\mu$  is mu,  $\nu$  is nu, and  $b$  is burgVectMod. The emission prefactor is called D0 . Loop.

The corrections applied to the migration energy of interstitials are the usual ones:

$$\Delta E_m(I) = \alpha_m[Ge] + \frac{1}{3} \sum_i^{x, y, z} \exp(-\Delta E_m^i/(k_B T)) \quad (717)$$

and for the binding of the particle to the loop is:

$$\Delta E_{b, loop} = P\Delta V_b^{loop} + \alpha_{loop}[Ge] \quad (718)$$

where  $\Delta V_b^{loop}$  is called VF . Loop, and  $\alpha_{loop}$  is called Alloy . Eb . Loop in the PDB.

Captured impurities (when Loop . Dopant . Model is true) re-emit impurities into the bulk with a frequency given by:

$$v_{emit}(A_i) = v_{0, emit}(A_i) \times \exp(-E_{emit}((A_i)/(k_B T))) \quad (719)$$

The prefactor and the activation energy are called D0.Loop and Eb.Loop in the PDB, respectively.

## Parameters

The parameters needed for the simulation of dislocation loops are defined for interstitials in silicon:

```
sprocess> pdbGet Si KMC I D0.311.To.Loop
1.6
sprocess> pdbGet Si KMC I E.311.To.Loop
0.68
sprocess> pdbGet Si KMC I D0.Loop
1000000.0
sprocess> pdbGet Si KMC I gamma
0.4375
sprocess> pdbGet Si KMC I mu
472
sprocess> pdbGet Si KMC I nu
0.3
sprocess> pdbGet Si KMC I Burger.Vector.Mod
0.3135
sprocess> pdbGet Si KMC I VF.Loop
0
sprocess> pdbGet Si KMC I Alloy.Eb.Loop
0
```

For impurity re-emission, the parameters are:

```
sprocess> pdbGet Si KMC In D0.Loop
200.0
sprocess> pdbGet Si KMC In Eb.Loop
2.0
```

**NOTE** These parameters can be changed to fit the dislocation loop formation and dissolution.

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Extended Defects

Figure 43 shows how a dislocation loop grows capturing interstitials, and how it shrinks recombining incoming vacancies or emitting interstitials.

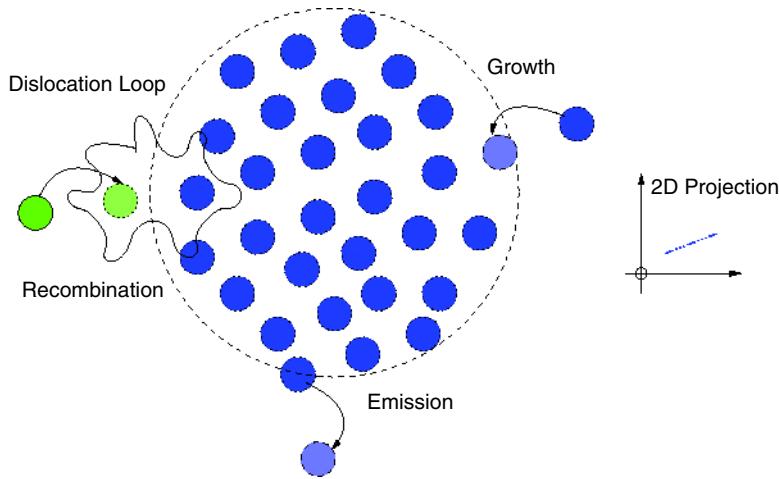


Figure 43 Emission, capture, and recombination of point defects in a dislocation loop

## Interactions

The interactions between dislocation loops and mobile particles are:

- Growth reactions. Only with neutral *I*s:

```
pdbSet Si KMC I ReactionsLoop I <true | false>
```

- Recombination reactions. Any vacancy:

```
pdbSet Si KMC I ReactionsLoop <V | VM | VP | VMM | VPP> <true | false>
```

- Impurity pairs break up and interact with the associated point defect (*I* or *V*). Only with pairs with the substitutional charge state the same as the substitutional dopant (for example,  $B_i^-$  for  $B^-$ ). The interstitial or vacancy is trapped or recombined, and the dopant is released (0) or trapped (1) depending on the model used. The model is specified for all dopants (default value) using the parameter Loop.Dopant.Model for interstitials.

This particular default can be overwritten for one particular dopant.

```
pdbSet Si KMC I Loop.Dopant.Model <true | false>
```

```
pdbSetDouble Si KMC <dopant> Loop.Dopant.Model <true | false>
```

## Parameters

Loops trap interstitials, but the recombination of vacancies is disabled:

```
sprocess> pdbGet Si KMC I ReactionsLoop  
I true
```

```
sprocess> pdbGet Si KMC V ReactionsLoop
V      false
```

Loops can break up some paired dopants, for example, boron:

```
sprocess> pdbGet Si KMC B ReactionsLoop
BiM    true
sprocess> pdbGet Si KMC I Loop.Dopant.Model
0
```

## Voids

Small vacancy defects have been reported (using paramagnetic resonance and photoluminescence) [20][21][22][23]. Theoretical studies [24][25] indicate that some of these small clusters can be particularly stable. Sentaurus Process KMC models these small clusters as APs and, consequently, they have irregular shapes. Nevertheless, size-dependent binding energies are considered for their V emission (see [Damage Accumulation Model: Amorphous Pockets on page 428](#)).

Vacancy clusters appear as spheroidal voids when they are big enough to be seen by TEM [26]. Tight-binding molecular dynamics studies show that the binding energies are a function of the cluster size [27] (see [Figure 44](#)).

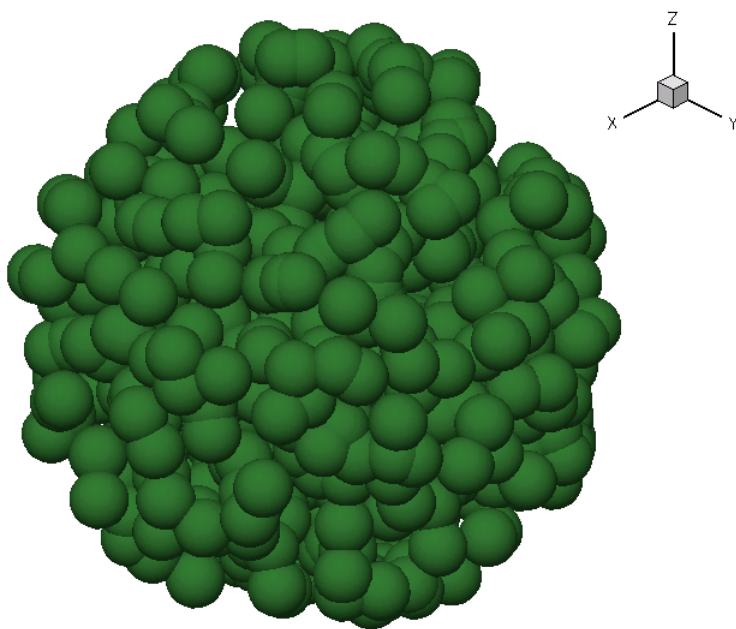


Figure 44 Voids are simulated with a spherical shape; this one contains 654 vacancies

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Extended Defects

## Shape

The threshold size between irregular small vacancy clusters (APs) and voids is specified with the parameter `Min.Void.Size`. Another parameter, `Max.Void.Diam`, is used to set up the maximum-allowed diameter (in nanometers) for these defects.

Reshaping the small clusters into voids above the mentioned limit is necessary to maintain the correct volume-to-surface ratio, as the V cluster grows. A large cluster of  $n$  vacancies is reshaped to be spheroidal, occupying the volume corresponding to the same number of silicon lattice sites. Sentaurus Process KMC manages the void shape to assert that its density is correct.

## Parameters

The parameters for voids are specified for silicon material and vacancy as species:

```
sprocess> pdbGet Si KMC V Min.Void.Size  
27  
sprocess> pdbGet Si KMC V Max.Void.Diam  
5.0
```

## Capture

Voids capture neutral vacancies, rearranging them to have a spheroidal shape. [Figure 45](#) shows the possible interactions between voids and point defects.

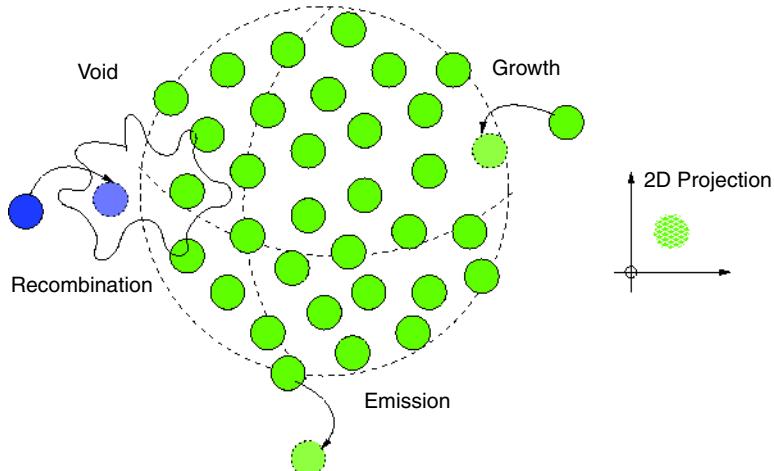


Figure 45 Voids are big cluster vacancies with a spherical shape that grow trapping neutral vacancies and shrink by recombination and vacancy emission

## Emission

Voids emit neutral vacancies with a frequency:

$$v = v_0 \times \exp(-(E_{b, void}(\text{size}) + \Delta E_{b, void} + E_m(V) + \Delta E_m(V))/(k_B T)) \quad (720)$$

$v_0$  is a prefactor that includes a constant and a dependency with the surface of the void, and  $E_{b, void}(\text{size})$  is the binding energy of a void. These binding energies are assigned in the parameter database together with the small vacancy-cluster binding energies. For information on how to locate and modify them, see [Amorphous Pockets Life Cycle on page 434](#). For voids, only the values for sizes bigger than the AP–void threshold apply.

Finally, corrections to the migration energy of vacancies and the binding of them to the void are applied. The migration correction is the usual one:

$$\Delta E_m(V) = \alpha_m[Ge] + \frac{1}{3} \sum_i^{x,y,z} \exp(-\Delta E_m^i/(k_B T)) \quad (721)$$

For the binding energy, it is corrected using the parameter for small vacancy clusters:

$$\Delta E_{b, void} = P \Delta V_b^{cluster}(V) + \alpha_{void}[Ge] \quad (722)$$

where  $\alpha_{void}$  is Alloy.Eb.Void.

## Recombination

Voids recombine incoming interstitials with any charge.

## Interactions

Interactions between void defects and other particles fall into these categories:

- Trapping of neutral vacancies (growth):

```
pdbSet Si KMC V ReactionsVoid V <true | false>
```

- Recombination of interstitials:

```
pdbSet Si KMC V ReactionsVoid <I | IM | IP> <true | false>
```

- Impurity pair breakup. Voids do not trap impurities, but they can trap or recombine the interstitial or vacancy associated with a paired impurity, for example,  $B_i + V_n \rightarrow B^- + V_{n-1}$ . The pair must have the same charge as the substitutional dopant (in other words,  $B_i^-$  for  $B^-$ ,  $AsV^+$  for  $As^+$ ).

```
pdbSet Si KMC <impurity> ReactionsVoid <species> <true | false>
```

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Amorphization and Recrystallization

#### Parameters

Voids trap vacancies and recombine interstitials:

```
sprocess> pdbGet Si KMC V ReactionsVoid  
V      true  
sprocess> pdbGet Si KMC I ReactionsVoid  
I      true
```

Voids may break up some pairs. For example,  $B_i^-$  is disabled:

```
sprocess> pdbGet Si KMC B ReactionsVoid  
BiM    false
```

---

## Amorphization and Recrystallization

A predictive atomistic process simulator must include an amorphization model. Nevertheless, accounting for each particle and position during the amorphization, although possible [28], is not convenient for the sizes, times, and computer resources involved in process modeling. Despite this, amorphization involves the destruction of the lattice structure. Without a lattice, the KMC method, which discards the lattice and tracks only defects, is opened to a quasiamolecular approach, as explained in this section.

[Figure 46](#) shows a generic damage concentration profile after an implantation.

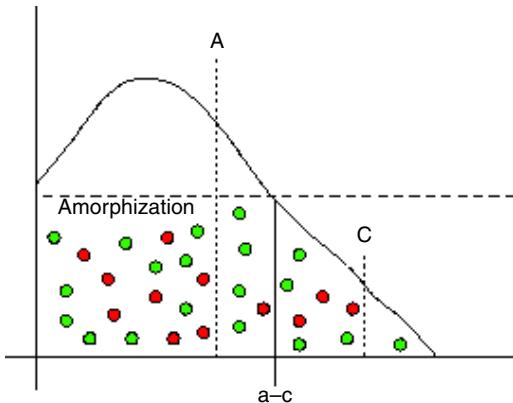


Figure 46 Damage concentration profile after an implantation

There are two different concentrations in [Figure 46](#) (A and C) and one concentration threshold called Amorphization. This threshold is stored in the parameter database in the damage section as Amorph.Threshold:

```
sprocess> pdbGet Si KMC Damage Amorph.Threshold  
1.5e+22
```

**NOTE** You can change this limit if necessary. The damage accumulation model is dependent on the Amorph.Threshold.

The behavior of the simulator while adding new point defects (damage) differs depending on the local concentration of the internal grid elements. A new point defect is inserted into a box depending on the concentration of that box. If the concentration is smaller than the Amorphization threshold (C, crystalline region), the point defect is inserted as it is. In other words, a particle is placed inside the simulator with its three coordinates, the defect, and the particle type. Finally, the damage concentration can be higher than the amorphization threshold (region A (amorphous) in [Figure 46 on page 450](#)). In this case, if a particular crystalline volume (specified by the parameter Min.Amorph.vol) has an averaged damage concentration larger than the threshold, the entire internal volume is assumed to be amorphous. The atomistic 3D coordinates for Is and Vs are discarded for amorphous boxes because the definition of a point defect is now meaningless in an amorphous region, and only their concentration is stored. Finally, the material of the internal box changes from crystalline (such as silicon) to amorphous (such as amorphous silicon) and an interface, which can simulate a three-phase segregation model, is created between them.

**NOTE** For amorphous regions, the atomistic 3D information is discarded, and only the number of particles is stored. When asking Sentaurus Process KMC for atomistic information (the 3D coordinates for each particle), you should not expect to obtain Is and Vs in amorphous regions.

**NOTE** To obtain the amorphous–crystalline interface, use the command:

```
kmc extract acinterface
```

---

## Amorphous Defects

An amorphous defect is a special defect assigned to each grid element of Sentaurus Process KMC with a damage level above the amorphization threshold.

### Material

Amorphous defects are always associated with amorphous materials. Each amorphous internal element is paired with an amorphous defect.

### Shape

The shape of an amorphous defect coincides with the element containing it. Amorphous layers are created as a set of several amorphous defects. Consequently, amorphous layers can follow

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Amorphization and Recrystallization

any complicated amorphous geometry, but always as a set of Sentaurus Process KMC elements.

## Growth

Amorphous defects do not grow because they are limited to the size of the element. Amorphous layers grow when new elements are amorphized and become amorphous. These amorphous elements capture any incoming particle.

## Recombination

These defects can recombine their damage and become crystalline silicon. Amorphous defects do not emit particles; recrystallization is the only event they can perform.

---

## Diffusion in Amorphous Materials

Two models are available for diffusion in amorphous materials:

- A simple direct diffusion model
- An indirect diffusion model that uses dangling bonds as an intermediate species

To select the model to use, set:

```
KMC <material> Damage Amorphous.Bonds true
```

where <material> is the crystalline material.

## Direct Diffusion Model

Dopants can diffuse in amorphous materials using direct diffusion. The implemented diffusivity is:

$$D_m(X) = D_{m,0}(X)\exp(-E_m((X)/(k_B T))) \quad (723)$$

The parameters  $D_{m,0}$  and  $E_m$  are input parameters. They are needed for diffusion in amorphous materials and are specified in the PDB as  $D_m$  and  $E_m$ , respectively, under the amorphized material:

```
pdbSet <amorphous material> KMC <dopant> Em <dopant> <value>
```

For example:

```
pdbSet AmorphousSilicon KMC B Em B 0.8
pdbSet AmorphousSilicon KMC B Dm B 1e-3
```

**NOTE** The alias `aSi` can be used for `AmorphousSilicon`.

## Indirect Diffusion Model

The observed boron diffusion in amorphous silicon does not seem to obey a standard Fick's law with constant diffusivity prefactors and activation energy, thereby making the direct diffusion model in amorphous silicon inaccurate. A different model has been proposed [29][30] that relies on the presence and distribution of dangling bonds and floating bonds, and that interacts with boron atoms. In this model, an initial number  $n_0$  of dangling bonds (threefold-coordinated atoms) and floating bonds (fivefold-coordinated atoms) is created during amorphization.

These dangling bonds and floating bonds are allowed to evolve using a simple direct diffusion  $D_d$  for dangling bonds and  $D_f$  for floating bonds. Dangling bonds and floating bonds can interact with them, annihilating each other. Dangling bonds also can interact with boron (or any other user-defined impurity) with a proportionality constant  $\alpha$ .

In this model, boron in amorphous silicon can exist in two different states: an immobile fourfold-coordinated  $B^4$  state and a highly mobile threefold-coordinated  $B^3$  state. Boron changes between these two states by capturing and releasing a dangling bond. The threefold mobile boron is allowed to diffuse with a simple Arrhenius plot. Boundary conditions can be set at the `AmorphousSilicon_Silicon` and `AmorphousSilicon_Oxide` interfaces for dangling bond (DB) and floating bond (FB) recombination. Finally, despite the initial concentration  $n_0$  of dangling bonds produced by amorphization, an extra contribution of  $\gamma[B]$  is added to produce a total DB concentration of:

$$n_B = n_0 + \gamma[B] \quad (724)$$

where  $\gamma$  is a coefficient relating to the presence of boron atoms in amorphous silicon with an excess of dangling bonds, and  $[B]$  is the concentration of boron in amorphous silicon.

Consequently, the following reactions are allowed:



## Implementation

To minimize the number of species and physical mechanisms, the implementation of indirect diffusion through dangling bonds and FBs has been done by renaming:

- Dangling bonds as *interstitials in amorphous silicon*
- Floating bonds as *vacancies in amorphous silicon*

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Amorphization and Recrystallization

- $B^4$  as *substitutional boron in amorphous silicon*
- $B^3$  as *interstitial boron in amorphous silicon*

In this way, all that is needed is to allow  $I$  and  $V$  inclusion, and the following reactions in amorphous silicon:



The  $B$  interaction with  $I$  and further emission by  $B_i$  are modeled as a regular kickout mechanism. Consequently, the parameter  $\alpha$  is modeled indirectly through the binding energy and prefactor of the  $B_i$  pair.

When amorphizing an element with volume  $\Delta V$ , an initial number of  $n_0 \Delta V \delta$   $I$ s and  $V$ s will be created inside, where  $\delta$  is the silicon density. If there are boron atoms inside or boron atoms are introduced through implantation or any other means (for example, using the `select` command or the `profile` command), an extra number of  $\gamma$   $I$ s will be introduced per boron atom.

### Parameters

The parameters needed for this model are introduced in different places. If you want to model the indirect diffusion of boron in amorphous silicon (other impurities or amorphous materials are accepted also), you can use `aSi` as an alias for `AmorphousSilicon`.

Table 59 Parameters used for indirect diffusion in amorphous silicon

Parameter	Description	Symbol
<code>aSi KMC amorphous.bond true</code>	Model activation.	None
<code>aSi KMC I Dm I &lt;value&gt;</code> <code>aSi KMC I Em I &lt;value&gt;</code>	Dangling bond diffusion.	$D_d$
<code>aSi KMC V Dm V &lt;value&gt;</code> <code>aSi KMC V Em V &lt;value&gt;</code>	Floating bond diffusion.	$D_f$
<code>aSi KMC B Dm Bi &lt;value&gt;</code> <code>aSi KMC B Em Bi &lt;value&gt;</code>	$B_3$ diffusion.	None
<code>aSi KMC B Eb Bi &lt;value&gt;</code> <code>aSi KMC B Eb Bi &lt;value&gt;</code>	$B_3$ - $B_4$ reaction rate.	$\alpha$
<code>aSi KMC B ReactionsPointDefect B,I true</code>	$B^4 + DB \leftrightarrow B^3$ .	None

Table 59 Parameters used for indirect diffusion in amorphous silicon

Parameter	Description	Symbol
Si KMC Damage Amorphous.n0 <value>	Initial dangling bond and floating bond percentage (versus silicon density).	$n_0$
aSi KMC B gamma <value>	Number of dangling bonds created per boron atom.	$\gamma$

## Impurity Clusters in Amorphous Materials

Impurities diffusing in amorphous materials can interact with each other and can form impurity clusters. In contrast with impurity clusters in crystalline volumes, amorphous impurity clusters do not contain interstitials or vacancies, and are only an agglomeration of impurities. Consequently, they can only re-emit the trapped impurities. With this exception, they behave like regular impurity clusters (see [Impurity Clusters on page 470](#)).

## Recrystallization

Different recrystallization models are implemented:

- One simple KMC model assigns a recrystallization rate to each amorphous defect for recrystallization simulations. No orientation dependencies are allowed.
- Two fully atomistic models use a lattice kinetic Monte Carlo (LKMC) method to simulate the evolution of the amorphous–crystalline interface. These models include orientation-dependent solid phase epitaxial regrowth (SPER) and facet formation.

The recrystallization model is set up with:

```
pdbSet <material> KMC Damage SPER.Model <model>
```

where:

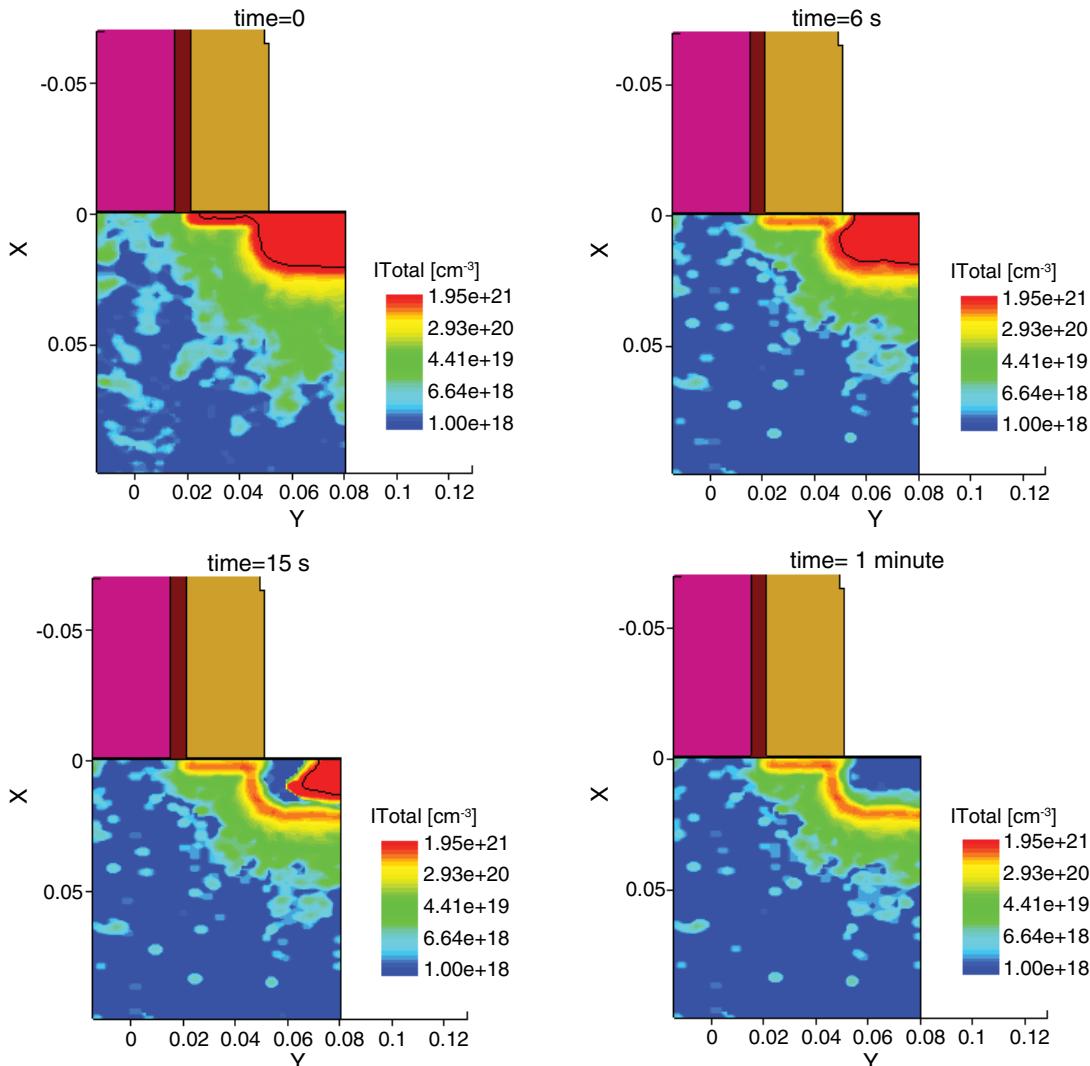
- <material> is the crystalline material (typically, silicon).
- <model> is one of the following:
  - KMC, a simple KMC model
  - LKMC or Planes, a basic LKMC model parameterized using the crystal orientation
  - Coordinations.Planes, an LKMC model that can be extended to account for local atomic configuration but currently is limited to parameterization using crystal planes, similar to the basic LKMC models

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Amorphization and Recrystallization

## KMC: Simple Solid Phase Epitaxial Regrowth

Recrystallization is implemented as a special event performed by the amorphous defects. At a given temperature, every amorphous defect can recombine all its internal damage, in other words, recrystallize, with a frequency  $v_{recrys}$ . The recrystallization of several amorphous defects with different recrystallization frequencies, depending on their recrystallization axis and the number of amorphous neighbors, generates an advancing recrystallization front, as can be seen in [Figure 47](#).



**Figure 47** Source and gate of a transistor during SPER as simulated by Sentaurus Process KMC. The total concentration of interstitials is represented during the evolution of the recrystallization front. At the end, there is damage only near the initial amorphous/crystalline interface. The remaining damage can form end-of-range (EOR) defects.

Therefore, if  $w$  is the length of an amorphous defect in the recrystallization direction, the frequency associated with the recrystallization is  $v/w$ . This recrystallization velocity  $v$  is computed as an Arrhenius function that includes dependencies on both the local Fermi level and the presence of impurities [31]:

$$V(n) = V_0^{Fermi}(n) \times \exp(-(E_{recrys}(n) + P\Delta V^{SPER} + c)/(k_B T)) \quad (729)$$

where:

- $E_{recrys}(n)$  parameters are specified as E.Recrys.
- $\Delta V^{SPER}$  is the activation volume for SPER (dependency on hydrostatic pressure) called VF.Recrys.
- $n$  is the percentage of amorphous material around a given element.

The time it takes to recrystallize an amorphous cell depends on the number of amorphous neighbors; the more neighbors that are amorphous, the longer it takes. The longer recrystallization takes, the more stable the amorphous defect, so its activation energy is bigger.

- $V_0^{Fermi}$  accounts for the prefactor, including dependency on the Fermi level. This dependency is introduced as:

$$V_0^{Fermi}(n) = V_0(n)(1 + |K \times \text{Doping}|) \quad (730)$$

being  $V_0(n)$  and the input parameter called V0.Recrys. Doping is the local amorphous element doping, and  $K$  is a calibration parameter (different for n-type and p-type materials) called V0.Recrys.ntype and V0.Recrys.ptype, respectively.

- $c$  takes into account the changes in SPER regrowth due to local impurity concentration. This correction term is modeled as:

$$c = \sum_{Impurities} (E_f(Impurity) - E_{recrys}(50)) \left( \frac{[Impurity]}{5 \times 10^{22}} \right)^x \quad (731)$$

The  $E_f(Impurity)$  parameter controls how much each impurity changes the planar recrystallization activation energy (assumed to have 50% amorphous neighboring elements).  $x$  is an exponent to control how this correction depends on the dopant concentration. A null impurity concentration gives a zero correction, while an impurity concentration of  $5 \times 10^{22}$  produces  $c = E_f(Impurity) - E_{recrys}(50)$ . Consequently,  $E_f(Impurity)$  represents the planar recrystallization activation energy if the sample contains only the impurity, while  $x$  allows it to control the transition between these two opposite situations. These parameters are called E.Recrys and E.Recrys.Exponent, respectively, in the PDB.

This model, in which elements with fewer amorphous neighbors recrystallize faster, extends the ideas described in the literature [28] for amorphous elements. This simple method can simulate the faster recrystallization of amorphous corners or thin amorphous panhandlers embedded in crystalline silicon.

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Amorphization and Recrystallization

Finally, if a recrystallization event that will break the compactness of the amorphous layer is detected, its recrystallization will be retarded by the parameter `Compact.Factor`. This prevents the formation of amorphous isolated islands and ensures a better compactness of the amorphous material.

### Parameters

The parameters for the recrystallization model are:

```
sprocess> pdbGet Si KMC Damage VF.Recryst
0
sprocess> pdbGet Si KMC Damage V0.Recryst
0      1.7e8
99     1.7e8
100    0
sprocess> pdbGet Si KMC Damage E.Recryst
0      1.72
15     1.72
40      2.7
70      2.7
95      3.3
99      5
```

The unspecified values between two specified ones are computed by linear interpolation.

The parameters controlling the Fermi level and impurity concentration dependencies are specified for each dopant (and material). For example, for boron, they are:

```
sprocess> pdbGet Si KMC B E.Recryst
2.7
sprocess> pdbGet Si KMC B E.Recryst.Exponent
1
```

### LKMC: Fully Atomistic Modeling of Solid Phase Epitaxial Regrowth

It is well known that the SPER velocity depends on the substrate orientation with approximate ratios of 20:10:1 for orientations (100), (110), and (111), respectively. For orientation (100), two different recrystallization frequencies have been identified, depending on the total crystalline first and second neighbor atoms, which signify whether it is a high or low crystalline growth region. In addition, the recrystallization of thin layers in fin transistors is shown as an ‘arrow tip’ shape formed by two (111) planes that slow down the SPER, leading to the formation of polycrystalline silicon in regions still not recrystallized.

The LKMC or Planes model, based on [32], introduces the lattice in the amorphous–crystalline (a-c) interface and assigns a recrystallization event to each atom there.

When an internal mesh element is detected to be amorphous as explained in [Amorphization and Recrystallization on page 450](#), the silicon lattice is recreated around it.

The `Coordinations.Planes` model, however, creates a lattice in the entire domain and initializes the atoms at the a-c interface. At the core, the `Coordinations.Planes` model uses the algorithms employed in the `Coordinations` model for epitaxy, which allow multiple types of species in the system. However, its flexibility in SPER is limited. The parameter settings for prefactors and energies for SPER for this model are the same as those for the `LKMC` or `Planes` model.

The lattice in all models takes into account the wafer orientation specified in the `init` command. Those lattice atoms belonging to crystalline elements are assigned a ‘crystalline’ flag, while those belonging to the amorphous element are assigned an ‘amorphous’ flag. This produces the initial amorphous–crystalline interface. At this point, even when the amorphous–crystalline interface still follows the contour of the internal mesh, it is formed by a set of individual lattice atoms.

From this point, different recrystallization rates are assigned to each atom at the interface. The interface is defined as the set of lattice atoms that, having an amorphous state, has at least one first neighbor with a crystalline state. Any other lattice atom that does not belong to this interface has a recrystallization rate of 0. This means that crystalline-lattice atoms have a zero probability of recrystallizing (because they are already crystalline).

In some cases where regular SPER is very slow, random nucleation and growth can produce polysilicon material [33] not simulated here. Inclusion of defective silicon created during SPER also is not simulated in the `LKMC` or `Planes` model. However, in the `Coordinations.Planes` model, twin defects can be simulated along the  $\langle 111 \rangle$ -directions (see [Defect Generation During SPER on page 464](#)).

For amorphous lattice atoms belonging to the interface (in other words, surrounded by at least one crystalline lattice atom), a SPER rate is assigned. The model assumes that an atom in the amorphous phase must form two undistorted bonds with its first neighbors in the silicon phase to become crystalline. For amorphous atoms close to a (001) surface, this happens naturally. For (011) surfaces, two adjacent amorphous atoms have to *cluster* together so that each atom has two undistorted bonds. Finally, for (111) orientations, three atoms are needed to cluster together.

Consequently, there will be three different recrystallization prefactors –  $K(1)$ ,  $K(2)$ , and  $K(3)$  – depending on the number of amorphous atoms needed to complete two undistorted bonds. These  $K(1)$ ,  $K(2)$ , and  $K(3)$  prefactors will be related but not proportional to the different (001), (011), and (111) SPER velocities. The prefactor  $K(1)$ , associated with the (001) orientation, can again be dependent on how many total first ( $c_{1NN}$ ) and second ( $c_{2NN}$ ) crystalline neighbor atoms are present. A low crystalline growth region is identified by  $c_{1NN} + c_{2NN} \leq 8$ , while a high crystalline growth region is identified by  $c_{1NN} + c_{2NN} > 8$  [34]. In particular,  $K(2)$  and  $K(3)$  are probabilities for two and three atoms, respectively, to come together in an

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Amorphization and Recrystallization

amorphous phase and form spontaneously undistorted crystalline bonds between them. Consequently, K(2) is expected to be smaller than K(1), and K(3) is expected to be smaller than K(2), by several orders of magnitude.

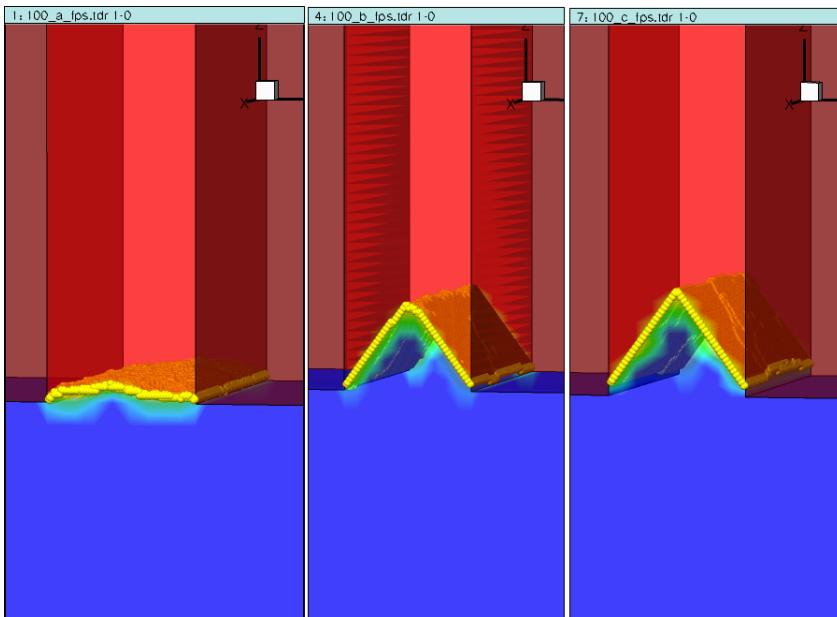
Each of these lattice atoms is given a recrystallization frequency of:

$$v^{\text{LKMC}} = v_0^{\text{Fermi}} \times K(n) \times \exp\left(-\frac{(E_{\text{recrys}}^{\text{LKMC}} + (|\epsilon_{xy}| + |\epsilon_{xz}| + |\epsilon_{yz}|)\lambda + P\Delta V^{\text{SPER}} + c)}{k_B T}\right) \quad (732)$$

$K_{(n)}$  are the K(1), K(2), and K(3) prefactors explained above where:

- $v_0^{\text{Fermi}} = 1 + |K \times \text{Doping}|$  is a Fermi-level correction similar to [Eq. 730](#).
- $E_{\text{recrys}}^{\text{LKMC}}$  is taken as  $E_{\text{recrys}}$ (50) in [Eq. 729](#).
- $|\epsilon_{xy}|$ ,  $|\epsilon_{xz}|$ , and  $|\epsilon_{yz}|$  are the absolute value of the shear stresses.
- $\lambda$  is a parameter coupling the shear stresses.
- $P\Delta V^{\text{SPER}}$  and  $c$  are the same terms as those defined in [Eq. 729](#).

[Figure 48](#) shows the evolution of an amorphized fin during SPER when this model is used, after 2-, 4-, and 6-minute annealings at 550°C .



[Figure 48](#) SPER evolution (blue is crystalline silicon; red is amorphous one) with time (*left to right*) 2, 4, and 6 minutes at 550°C of a thin (20 nm) silicon fin. The oxide (brown material) does not provide the correct template for the lattice atoms to form undistorted bonds, stopping the recrystallization and leading the way to the (111) planes. When the two (111) planes are formed, no further fast (100) SPER is possible, and the SPER occurs through the very slow and defect-prone (111) recrystallization.

When the arrow tip is formed by the two lateral (111) planes, the recrystallization is almost stopped (*middle* and *right* images). The planes are formed by the presence of the oxide–silicon interface. Since the oxide does not provide the needed undistorted bonds for silicon recrystallization, it is used as a starting point for the (111) plane formation.

A similar model using LKMC for epitaxial regrowth is described in [Chapter 6 on page 567](#).

Several corrections are applied to the recrystallization rate of a lattice atom. Three of them – the pressure correction ( $P\Delta V^{\text{SPER}}$ ), the impurity correction (through the term  $c$ ), and the Fermi-level correction ( $v_0^{\text{Fermi}}$ ) – are the same in both this model and the simple KMC model (see [KMC: Simple Solid Phase Epitaxial Regrowth on page 456](#)).

### Stress Correction

Stress correction for the calculation of recrystallization frequencies has been adopted from [34]. This stress correction is applied when you set **KMC Stress 1**. The recrystallization frequency on stress becomes:

$$v(T, \sigma) = v_0 \times \exp\left(\frac{V_{ij}\sigma_{ij}}{k_B T}\right) \quad (733)$$

where:

- $\sigma_{ij}$  is the stress state.
- $V_{ij}$  is the activation volume (or strain tensor) that can be represented in terms of normalized regrowth direction,  $d(n)$ , and the parallel and perpendicular components of the activation strain tensor,  $V_{\parallel}$  and  $V_{\perp}$ , by the following relation:

$$V_{ij} = V_{\parallel}d_i d_j + V_{\perp}(\delta_{ij} - d_i d_j) \quad (734)$$

where  $\delta_{ij}$  is the Kronecker delta, and  $d_i$  and  $d_j$  are the Cartesian components of the normal vector  $d(n)$ .

$V_{\parallel}$  and  $V_{\perp}$  are the only parameters needed for this model. According to [34], these two components of the activation strain tensor depend on the first crystalline nearest neighbors. See the **VD.Recryst** parameter in [Table 60 on page 463](#).

### Shear-Strain Correction

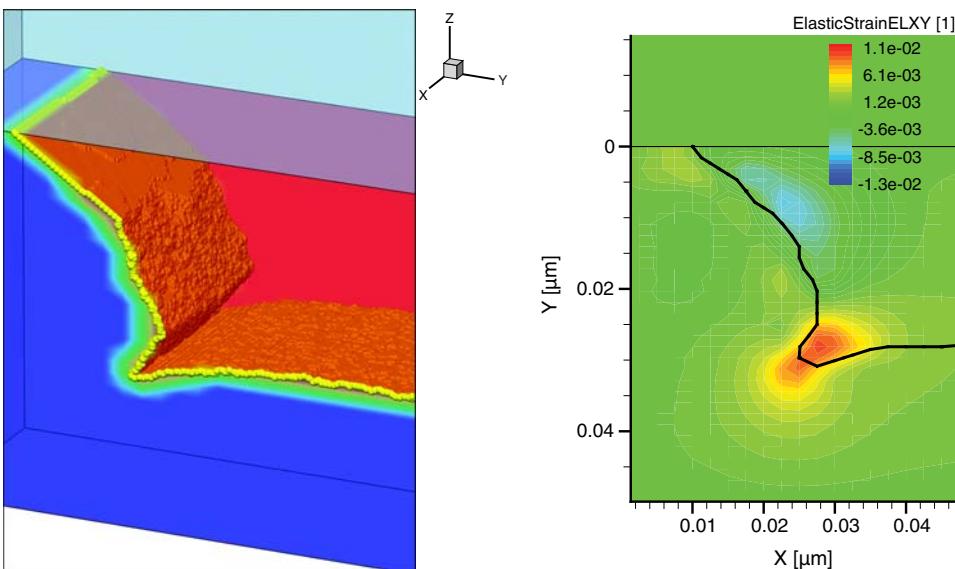
The correction for shear strain,  $(|\epsilon_{xy}| + |\epsilon_{xz}| + |\epsilon_{yz}|)\lambda$ , is unique to this model. Its inclusion allows the LKMC models to successfully simulate the evolution of line-shaped amorphized regions. The experimental rate at the corners of line-shaped amorphized regions is very small, producing a pinching of the SPER interface at the corners [35]. This can be simulated with the inclusion of this shear stress term [32]. The shear strain is generated during amorphization due to the different density of the amorphous phase. The expansion of the amorphous phase is not

## 5: Atomistic Kinetic Monte Carlo Diffusion

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possible in embedded amorphous regions. The compression of the amorphous phase leads to a sharp gradient of shear stress at the corners. The model uses the shear strain to simulate the anomalous regrowth patterns and facet formation experimentally seen in rectangular-shaped amorphized regions, as shown in [Figure 49](#).

[Figure 49 \(left\)](#) shows the distribution of lattice atoms at the amorphous interface side. A (111) plane, featuring a small nano-island, can be observed close to the interface. The trench formed at the corner is due to the perturbation introduced by shear strain. [Figure 49 \(right\)](#) shows the xy shear strain distribution; its maximum intensity occurs at the corner.



**Figure 49** Recrystallization of a rectangular-shaped amorphous region using the LKMC model

Since this model relies on the strain created by the different density of the amorphous material versus the silicon one, some extra commands must be introduced in the script to account for it.

First, a new material to account for amorphous silicon in the mechanics simulator must be introduced:

```
mater add name= Amorph
```

Mechanics properties for this new material must be defined:

```
pdbSetDoubleArray Silicon Amorph Conc. Strain {0 0 1 0.02}
pdbSetBoolean      Silicon Mechanics UpdateStrain 1
```

and Sentaurus Process KMC must be instructed that stress is being taken into account:

```
pdbSet KMC Stress 1
```

Finally, the synchronization between the atomistic and the mechanics simulator is automatic. After every mechanics step, the KMC Stress 1 parameter instructs Sentaurus Process KMC to update the stress and strain fields. After each diffusion (atomistic diffusion) step, Sentaurus Process KMC updates the Amorph distribution by automatically calling the procedure KMCSync written in the KMC.tcl file.

This procedure, which can be modified by users but, in principle, does not need to be, contains the lines responsible for updating the amorphous region in mechanics to properly account for the strain and stress:

```
LogFile IL2 "A/C synchronization: KMC -> PDE"
kmc deatomize name=AC
sel Silicon z=1e22*AC name=Amorph store
```

**Table 60** lists the parameters used in the LKMC model. It is assumed that silicon (Si) is the crystalline material and amorphous silicon (aSi) is the amorphous material.

Table 60 Parameters for LKMC model

Parameter name in parameter database	Description	Symbol
Si KMC Damage SPER.Model <model>	Sets the model to use. Either LKMC, or Planes, or Coordinations.Planes. Use KMC for quasiamolecular simulations.	None
Si KMC Damage SPER.Model.100 <model>	Options are: <ul style="list-style-type: none"> <li>• Isotropic applies a uniform prefactor along the (001) direction.</li> <li>• Planar applies different prefactors along the (001) direction depending on whether it is a low or high crystalline growth region.</li> </ul>	None
Si KMC Damage SPER.Model.111 <model>	Options are: <ul style="list-style-type: none"> <li>• Isotropic applies a uniform prefactor along the (111) direction.</li> <li>• Twin.Assisted uses the same prefactors as Isotropic, but it allows for possible twinning of the lattice.</li> </ul>	None
Si KMC Damage prefactor.SPER.100 <value>	Value for the prefactor associated with 100 SPER for Isotropic model.	K(1)
Si KMC Damage prefactor.SPER.100.7 <value>	Value for the prefactor associated with 100 SPER for Planar model for low crystalline growth region.	K(1)
Si KMC Damage prefactor.SPER.100.8 <value>	Value for the prefactor associated with 100 SPER for Planar model for high crystalline growth region.	K(1)
Si KMC Damage prefactor.SPER.110 <value>	Value for the prefactor associated with 110 SPER.	K(2)
Si KMC Damage prefactor.SPER.111 <value>	Value for the prefactor associated with 111 SPER.	K(3)
Si KMC Damage Shear.Coupling <value>	Shear-strain coupling parameter.	$\lambda$

## 5: Atomistic Kinetic Monte Carlo Diffusion

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Table 60 Parameters for LKMC model

Parameter name in parameter database	Description	Symbol
Si KMC Damage VF.Recryst <value>	SPER pressure correction (same as the KMC model).	$\Delta V^{\text{SPER}}$
Si KMC Damage VD.Recryst <values>	Array parameter, depending on the number of crystalline first neighbors, related to the atomic volume of the material.	$\text{m}^3/\text{mol}$
Si KMC Damage E.Recryst 50 <value>	Activation energy for recrystallization (same as the KMC model).	$E_{\text{recryst}}^{\text{LKMC}}$
Si KMC Damage V0.Recryst.ntype <value> Si KMC Damage V0.Recryst.ptype <value>	Fermi-level corrections (same as the KMC model).	$v_0^{\text{Fermi}}$
Si KMC Damage E.Recryst <value> Si KMC Damage E.Recryst.Exponent <value>	Impurity corrections (same as the KMC model).	$c$
Si KMC Damage Lattice.Constant <value>	Lattice constant.	None

## Defect Generation During SPER

It is known that when (111) planes have formed in a simulation, the recrystallization beyond these planes is defective, and silicon of low quality, or even polysilicon, is formed. In the LKMC or Planes model, a simple predictive model for defect formation during SPER based on [36] and [37] is included. However, in the Coordinations.Planes model, lattice twinning can be modeled as well, based on [38].

### LKMC Model or Planes Model

Such modeling is performed by assigning two tags after every recrystallization event in the lattice: a *normal* tag for sites sharing the substrate configuration, and a *defective* tag for sites assumed not to bond to their neighbors and that form twin defects. Although this modeling does not physically set the atoms in twin positions, but only assigns them a *tag* while remaining in a perfect crystalline position, it is sufficient to predict the defective regions in silicon and to slow down SPER in a similar way to experiments [36][37].

The new defective sites are produced by two mechanisms:

- Recrystallization of (111) sites, having a probability Pdef of becoming defective.
- Recrystallization of atoms in the neighborhood of defective sites, inheriting such tags and becoming also defective.

The definition of a coordination number, a keystone in this model to identify the microscopic configurations, also is modified to distinguish between normal and defective sites. In this way, the formation of defects slows down the recrystallization of neighboring sites.

The formed defects are represented in the non-LKMC module as an *IV twin defect* in the TDR file. No actions are associated with them in the regular KMC simulator. Consequently, when they are formed, twin defects do not disappear and do not interact with other particles. They are created for users to identify the regions predicted to have highly defective silicon.

The only new parameter needed for the model is the probability of (111) recrystallizations to produce twin defects. This parameter is specified in:

```
pdbSet KMC Si Damage probability.SPER.defect <0-1>
```

[Figure 50](#) and [Figure 51 on page 466](#) show two examples where twin-defect formation is involved. [Figure 50](#) represents the formation of defects during the SPER of a thin silicon fin. [Figure 51](#) shows the defective triangular-shaped region, bounded by a (111) plane, typical of SPER close to  $\text{SiO}_2$ -filled trenches.

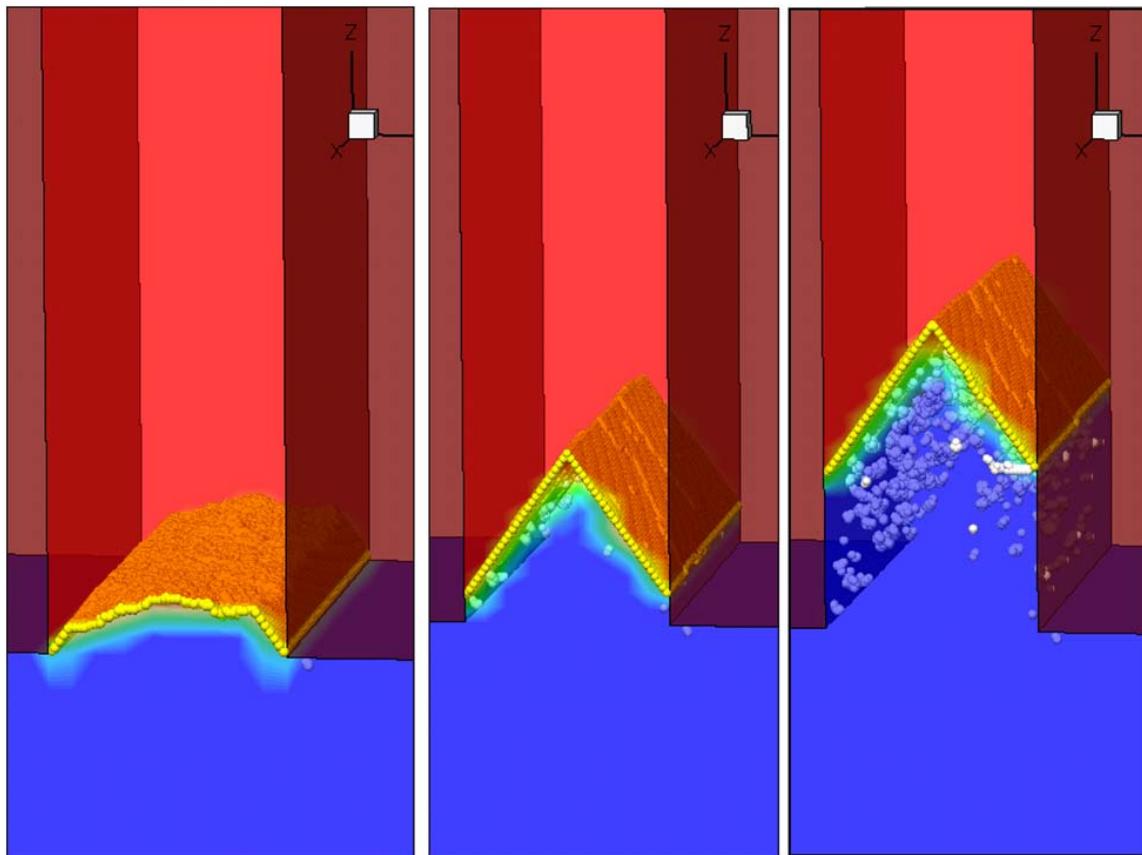


Figure 50 Evolution of a thin (20 nm width) amorphized silicon fin (amorphous is red, crystalline is blue) annealed at 600°C; arrow-shaped a/c interface is represented by yellow atoms and formation of defects (twins) is shown as white spheres

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Amorphization and Recrystallization

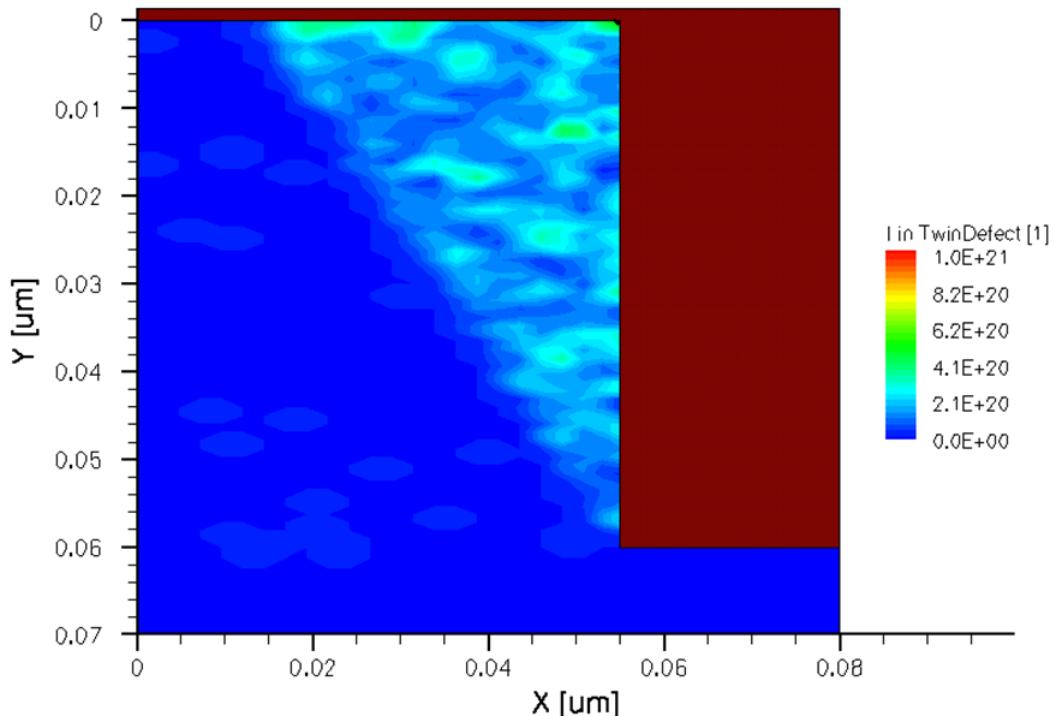


Figure 51 Concentration of twin defects representing defective silicon formation when SPER is in an amorphous region close to  $\text{SiO}_2$  (silicon is blue,  $\text{SiO}_2$  is brown)

### Coordinations.Planes Model

The `Coordinations.Planes` model allows crystal twinning along  $<111>$  directions and, therefore, the formation of low-quality crystalline silicon. To enable twinning along  $<111>$  directions, you should also set:

```
pdbSet Si KMC Damage SPER.Model.111 Twin.Assisted
```

It uses the same defect probability specified by:

```
pdbSet KMC Si Damage probability.SPER.defect <0-1>
```

Similar to the `LKMC` or `Planes` model, the SPER plane is determined by looking at the number of crystalline first nearest neighbors. When an atom in the  $<111>$  plane is being crystallized, the local growth direction is estimated by taking the difference between the coordinates of the atom being crystallized and its only crystalline first nearest neighbor. A random number is chosen to identify whether a twinning event will occur, based on the defect probability given by users. After this atom is crystallized, a new set of nearest neighbor amorphous atoms is either created in the original lattice sites or at twinned lattice sites, chosen according to the local growth direction.

By default, at the end of the diffusion step, all the crystallized atoms are cleaned. Only atoms near the a-c interface will be visible when loading the TDR file. To save information about the crystallization of atoms along twinned directions in the TDR file, enable visualization of these twinned grain orientations using the following setting:

```
pdbSetBoolean LKMC SPER.Cleanup false
```

This setting does not clean the atoms in the crystallized region at the end of the diffusion step, and so you can visualize them along various twinned directions.

## Redistributing Damage

The recrystallization event forces all *IV* pairs inside an amorphous defect to recombine. The *I* or *V* excess is redistributed to the neighboring amorphous boxes if any. Otherwise, the excess is recombined at the surface. If there are no free surface or interface neighboring amorphous boxes, it is left as point defects. If the recrystallization front has crossed several elements, the amount of excess point defects can be high. When the defects are deposited in the crystalline silicon, they grow and ripen into extended defects depending on the annealing conditions.

### Parameters

The parameter `Deposit.Excess.Damage` controls whether to redistribute the excess or to discard it. In simulations with buried amorphous layers, setting this parameter to `true` is suggested:

```
sprocess> pdbGet Si KMC Damage Deposit.Excess.Damage  
0
```

## Impurity Sweep/Deposit

The recrystallization process may affect the impurity concentration. The recrystallization front moves indium and other dopants away, changing the concentration profiles [39][40]. To model this effect, the amorphous defects transfer impurities during recrystallization:

- Dopants usually (`recrysDeposit`) remain in the box or move away with the recrystallization front (see [Figure 52 on page 468](#)). The available models for this movement are `Elements` and `Hops`, chosen by the `Redistribution.Model` parameter:
  - The `Elements` model takes all the *n* particles in one internal element and moves *n* × `Recryst.Deposit` to the adjacent one. If moving the dopant with the recrystallization front increases the concentration of the neighboring element more than a limit (`Recryst.Max.Total`), it will be deposited in the current element, no matter what its moving probability.
  - The `Hops` model goes particle-by-particle inside the affected element and decides whether the particle should be displaced a second neighbor distance, depending on

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Amorphization and Recrystallization

`Recryst.Deposit`. If the particle is not displaced, it remains where it was. The algorithm continues with the next particle (which may still be the same one, pushing it again through the adjacent element little by little) until no more particles remain. To prevent the concentration of displaced particles being too high, the algorithm forces the deposit probability to be 1 when a particle has 25 or more dopant neighbors. The algorithm corrects this probability by linear interpolation starting when the number of neighbors is given a percentage of 25. This percentage is controlled by the parameter `Recryst.Deposit.Threshold`.

- When the box is recrystallized, if the remaining dopant concentration is bigger than the solubility limit (`C0.Recryst.Max.Active`, `E.Recryst.Max.Active`) after SPER, the extra dopants are deposited as impurity clusters. These clusters have a limited size, and there are two different models to deposit these clusters depending on whether `Recryst.Max.Size` is defined.

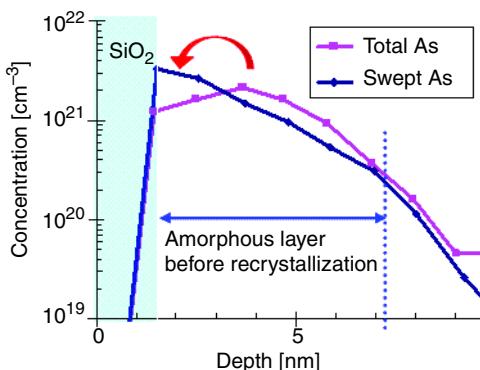


Figure 52 Impurity sweep example showing that arsenic has been pushed through the surface during recrystallization or SPER

The parameters for the recrystallization model are defined only for impurities in silicon (or other full material). `Pref.RecrystDeposit` and `Ener_RecrystDeposit` define (prefactor and energy) the probability for a dopant remaining in the same box after the recrystallization front passes. Setting this value to 1 disables the sweep of impurities. `Recryst.Max.Total` establishes the maximum concentration piled up during SPER. `Recryst.Max.Active` is the maximum-allowed concentration of an active dopant in recrystallized areas. Finally, if `Recryst.Max.Size` is defined (and it is by default), the old model to limit the maximum size of the deposited impurity clusters will be used. To undefine this parameter, use:

```
sprocess> pdbUnSetDouble Si KMC B Recryst.Max.Size
```

This instructs Sentaurus Process KMC to use the new model to deposit impurity clusters after SPER. This model deposits the clusters specified in `Recryst.Deposit.Complex` with the probabilities defined there.

Finally, the active dopants after SPER are deposited as substitutional impurities, but you can change this default using `Recryst.Deposit.Active`. This parameter accepts a list of impurities and impurity pairs with the probability to be deposited. For example:

```
sprocess> pdbSet Si KMC F Recryst.Deposit.Active F .1
sprocess> pdbSet Si KMC F Recryst.Deposit.Active Fi .9
```

This deposits 90% of the ‘active’ fluorine as `Fi`, and 10% as `F`.

**NOTE** Specifying a high probability for a cluster with a number of dopants greater than 1 does not necessarily mean that you will obtain only that cluster. For example, if you specify that  $B_2I$  should be 100% of the deposited clusters, but Sentaurus Process KMC finds only one boron particle in an element, Sentaurus Process KMC will not form a  $B_2I$ .

**NOTE** In the new model, that is, when `Recryst.Max.Size` is not set, low values of dopant activation (set by `C0.Recryst.Max.Active` and `E.Recryst.Max.Active`) may not be resolved properly. It is recommended to set `Fix.recrysMaxActive` to `true`, to resolve such low values of dopant activation levels during SPER. To set it, use:

```
pdbSet KMC Fix.recrysMaxActive true
```

## Parameters

The recrystallization parameters for dopants can be obtained as:

```
sprocess> pdbGet Si KMC As Pref.RecrystDeposit
0.3
sprocess> pdbGet Si KMC As Ener.RecrystDeposit
0.0
sprocess> pdbGet Si KMC As Recryst.Max.Active
1e+21
sprocess> pdbGet Si KMC As Recryst.Max.Size
4
sprocess> pdbGet Si KMC B Recryst.Deposit.Complex
B3I3 .40 B2I3 .30 BI2 .30
sprocess> pdbGet Si KMC B Recryst.Deposit.Active
B 1.0
```

To see which model is being used, use:

```
sprocess> pdbGet Si KMC Damage Redistribution.Model
Elements
```

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Impurity Clusters

The concentration thresholds associated with each model are:

```
sprocess> pdbGet Si KMC B Recryst.Max.Total  
2e+22  
sprocess> pdbGet Si KMC B Recryst.Deposit.Threshold  
75
```

---

## Impurity Clusters

At certain concentrations, dopants are electrically inactive in crystalline silicon [7]. At the same time, high  $I$  concentration can make a fraction of boron electrically inactive even when its concentration is below its solubility [41]. These phenomena can be explained by a  $B_mI_n$  clustering mechanism [15][42] or dopant precipitation [7]. Sentaurus Process KMC considers these mechanisms, implementing impurity clusters.

Studies [43] have shown that boron precipitation in amorphous silicon occurs through formation of a boron complex, thereby making the inclusion of impurity clusters in amorphous materials necessary. Consequently, pure dopant clusters,  $B_n$ , are allowed in amorphous materials and other materials modeled as simple.

The  $A_nB_o...X_m$  impurity clusters allow powerful modeling of the interaction of several impurities between them. For example, fluorine–boron clusters ( $F_nB_oI_m$  and  $F_nB_oV_m$ ) can be tried to explain the effects of boron coimplanted with fluorine, or  $As_nP_oV_m$  clusters to allow a satisfactory explanation, as seen in [53]. Nevertheless, the most common use of impurity clusters is the traditional one where only one dopant is present. Consequently, except where indicated, the description of impurity clusters that follows assumes that the clusters are in the more common form  $A_nX_m$  with only one impurity involved. Impurity clusters have a simple model for diffusion, that is, they can migrate (see [Diffusion of Impurity Clusters on page 472](#)).

Finally, impurity clusters do not need to be neutral. Consequently, the charge state of each impurity cluster can be defined using the parameter  $e0.Complex$ . When needed, an impurity cluster with a particular charge such as  $A_nX_m^{charge}$  will be denoted. In addition, clusters can react with charged particles, as long as the reaction is not between a cluster and a particle with the same sign, in other words, it is not an electrostatic repulsive reaction.

To simplify the following descriptions, this section describes  $A_nX_m$  clusters with only one impurity and neutral reactions (that is, reactions similar to  $A_nX_m^a + AX^b \leftrightarrow A_{n+1}X_{m+1}^c$ ,  $a + b = c$ ). To see how the model works when this is not the case, see [Charge Dependency on page 483](#).

**NOTE** Since P is used both for *positive* and *phosphorus*, clusters containing phosphorus cannot have P at the end of the cluster name. For example, AsIP will be interpreted as an arsenic–interstitial positive, while AsPI or PAsI will be an arsenic–phosphorus–interstitial cluster; the same is true for AsP, PAs, and so on.

## Shape of Impurity Clusters

An impurity cluster is an irregular agglomeration of impurities (A, B, ...) with or without interstitials and vacancies (X) that can be written as  $A_nB_o...X_m$ , with n impurity atoms of type A, o of type B, and so on, and m Is or Vs. If m = 0, it is a pure impurity cluster (the only ones allowed in simple materials).

For Sentaurus Process KMC, the notation  $A_nB_o...X_m$  means any possible configurations with n impurities of type A, o of type B, and so on, and m interstitial (vacancy) atoms. The interstitial (vacancy) atoms can be both silicon self-interstitials or dopant atoms in an interstitial position. Since Sentaurus Process KMC assumes all the  $A_nB_o...X_m$  configurations to be the same with only one effective formation energy, A, B, ... are represented always as a substitutional but inactive dopant or impurity, and X as a silicon interstitial or vacancy.

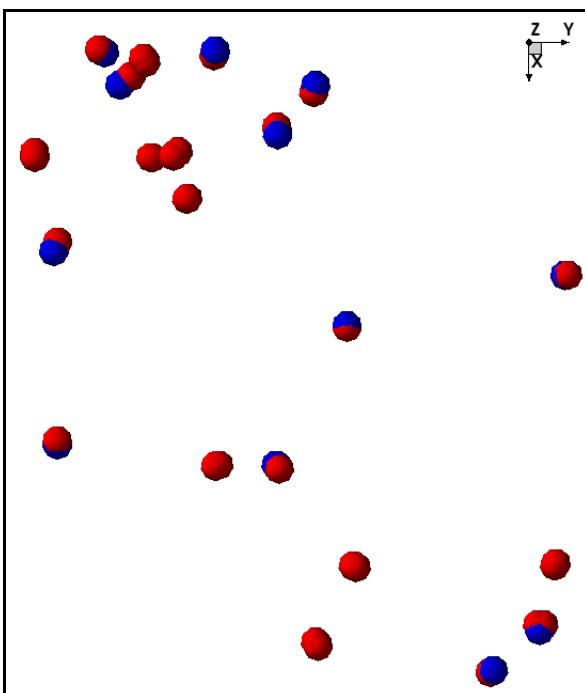


Figure 53  $\text{Bi}_2$  impurity clusters created using Sentaurus Process KMC; blue is boron and red is interstitial

---

## Diffusion of Impurity Clusters

A diffusion mechanism is available for impurity clusters, in which impurity clusters can perform migration hops similar to the ones performed by point defects, impurities, and dopants. An impurity cluster migration event involves all its constituent particles: The entire cluster is displaced. The particle coordinates are modified isotropically at a fixed distance of  $\lambda = 0.384$  nm in the orthogonal direction (parallel to the x-axis, y-axis, or z-axis).

The migration rate for impurity clusters is assumed to be:

$$v_m = v_{0,m} \times \exp(-E_m/k_B T) \quad (735)$$

where:

- $v_{0,m}$  is the prefactor for each cluster.
- $E_m$  is the migration energy for each cluster.

These diffusion parameters for impurity clusters are called `Dm.Complex` (prefactor) and `Em.Complex` (migration energy) in the PDB:

```
sprocess> pdbGet Si KMC As Dm.Complex As2V
1e-3
sprocess> pdbGet Si KMC As Em.Complex As2V
1.5
```

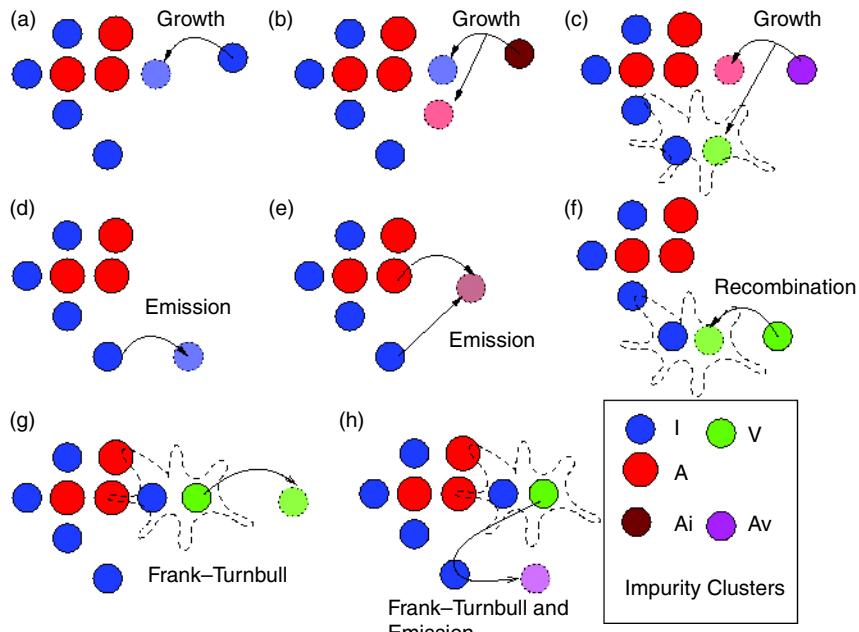
## Limitations of Diffusion

The migration events for impurity clusters, although similar to the ones for *single* particles, do not share all their features. In particular, the following limitations apply:

- The diffusivity of impurity defects is global, isotropic, and constant. There are no SiGe, stress, strain, or charge dependencies on diffusivity.
- Impurity defects do not interact with interfaces at all (Si–SiO<sub>2</sub> and so on). All interfaces are considered mirrors.
- Periodic boundary conditions or mirror conditions are correctly applied to the limits of the simulation box.
- There is no recombination probability at the boundaries. This means that the parameters `sinkProbTop`, `sinkProbBottom`, `sinkProbBack`, `sinkProbFront`, `sinkProbLeft`, and `sinkProbRight` do not apply to diffusing impurity clusters.
- Speedup migration does not apply to impurity cluster diffusion: no long hops or double hops.

## Growth of Impurity Clusters

Impurity clusters grow trapping neutral mobile particles (see [Figure 54](#)).



**Figure 54** Impurity clusters are disordered agglomerations of dopants and silicon point defects that trap and emit particles; Frank–Turnbull mechanisms and IV recombinations also are possible (light colors represent the reaction product, for example, light red and light blue in (b) represent the A atom and interstitial incorporation after  $A_i$  splits into A and I)

For an  $A_nI_m$  cluster, both  $I$  and  $A_i$  particles can be trapped:



The trapping is not automatic as it was for extended defects. In extended defects, the binding energy is always positive, so trapping is always allowed. For impurity clusters, the cluster can grow in both  $I_s$  (Vs) or dopants. The energy between the initial and final states is not always favorable. Sentaurus Process KMC computes the probability for an impurity cluster  $A_nI_m$  to trap an  $I$  or  $A_i$  as:

$$P_{\text{capture}} = \exp\left(-\frac{E_{\text{capture}}}{k_B T}\right) \quad (737)$$

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Impurity Clusters

where:

- $E_{\text{capture}}^{A_n I_m} = E_{\text{barrier}}(A_n I_m) + \max(0, E_b^{A_n I_m})$ .
- $E_{\text{barrier}}(A_n I_m)$  is an optional energy barrier.

The binding energies  $E_b^{A_n I_m}$  are computed using the potential impurity cluster energies:

$$\begin{aligned} E_b^{A_n I_m}(I) &= E_{\text{pot}}(A_n I_{m+1}) - E_{\text{pot}}(A_n I_m) \\ E_b^{A_n I_m}(A_i) &= E_{\text{pot}}(A_{n+1} I_{m+1}) - (E_{\text{pot}}(A_n I_m) + E_{\text{pot}}(A_i)) \end{aligned} \quad (738)$$

The potential energy for the neutral  $A_i$ , assuming that the substitutional  $A$  is negative, is given by  $-E_b(A_i^-) - e(-, 0)(A_i)$ , where the binding energy includes the pressure and Ge corrections. The minus sign accounts for the fact that the binding must have a sign that is opposite that of the potentials.

These potentials energies are computed as:

$$E_{\text{pot}}(A_n I_m) = E_{\text{pot}}^0(A_n I_m) + P \Delta V_{\text{pot}}(A_n I_m) \quad (739)$$

where:

- $E_{\text{pot}}^0(A_n I_m)$  is specified in the parameter database for each impurity in silicon as `Etotal.Complex`.
- $\Delta V_{\text{pot}}(A_n I_m)$  is the activation volume to take into account the hydrostatic pressure dependency, also defined for each impurity cluster size as `VF.Complex`.

The energy barriers are called `EbarrierIV.Complex` and `EbarrierDopant.Complex`. The `EbarrierIV` is defined for emission and capture of interstitials and vacancies, and `EbarrierDopant` for dopants or paired dopants.

For example, to set the potential energy of a BIC, such as  $\text{BI}_2$  to some value:

```
pdbSet Si KMC B Etot.Complex BI2 <n>
```

and, for  $\text{As}_4\text{V}$ :

```
pdbSet Si KMC As Etot.Complex As4V <n>
```

## Initial Seeds

The clusters  $A_2I$ ,  $AI_2$ ,  $A_2I_2$ , and  $A_2$  are the initial seeds for the impurity cluster ripening. The formation of  $A_2$  is discussed in [Percolation on page 475](#). The others are formed by the reactions:

- $A^a + A_i^b \leftrightarrow A_2I^c$
- $A_i^a + I^b \leftrightarrow AI_2^c$

- $A_i^a + A_i^b \leftrightarrow A_2I_2^c$
- $A^a + A^a \leftrightarrow A_2^c$

where  $a$  and  $b$  are the charge states for the reactants, and  $c$  for the result. All these reactions provide a cluster starting with impurities or impurity pairs. In cases where  $a + b \neq c$  for the first reaction or  $2a \neq c$  for the last one, the reaction is not neutral and the special considerations of [Charge Dependency on page 483](#) should be taken.

These initial seeds can be enabled or disabled independently using the parameter `ReactionsPointDefect` (see [Enabling and Disabling Interactions on page 418](#)).

## Percolation

Some dopants deactivate without visible diffusion when they are in high concentrations [44]. They also can form impurity clusters [45]. Sentaurus Process KMC models this deactivation allowing the substitutional dopants to interact with impurity clusters or with other dopants immediately after its inclusion in the simulation (for example, after being implanted or selected).

Arsenic can react with arsenic giving  $As_2$ . Substitutional As does not migrate, so this reaction is only possible when two arsenic atoms are close enough to each other. The higher the arsenic concentration, the higher this possibility. An  $As + As_2$  reaction and  $As_3 + As$  reaction also are possible. These species also are immobile. They react only when they are close enough. Consequently, the probability of forming an  $As_4$  cluster using this mechanism is low because it needs four As atoms close enough to each other. This probability increases with the concentration. With high concentration, the probability is not negligible, and the substitutional As react with each other forming As clusters and becoming inactive.

**NOTE** The reaction between two substitutional dopants to give an impurity cluster is the only exception to the rule that two particles with the same charge will not interact.

In simple materials, such as amorphous silicon, this percolation model is the only one allowing impurity clusters to be formed. Since all particles are neutral in simple materials, the percolation reaction does not constitute an exception there.

## Parameters

The potential and binding energies for impurity clusters are defined only in materials defined using the `full` and `simple` models, including amorphous. They are defined in arrays whose index is the cluster name. For example, for F clusters:

```
sprocess> pdbGet Si KMC F Etot.al.Complex
FV2      -4.20
```

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### Impurity Clusters

F2	-0.5	F2V	-4.63	F2V2	-7.07
F3	-1	F3V	-7.08	F3V2	-9.04
F4	-1.5	F4V	-7.12	F4V2	-11.47
F5	-3	F5V	-8.5	F5V2	-13.29
F6	-4.5	F6V	-9.7	F6V2	-16.09
		F7V	3		
				FI2	-4.20
		F2I	-4.63	F2I2	-7.07
		F3I	-7.08	F3I2	-9.04
		F4I	-7.12	F4I2	-11.47
		F5I	-8.5	F5I2	-13.29
		F6I	-9.7	F6I2	-16.09
		F7I	3		

A particular value for only one element also can be obtained. The current potential energy for  $\text{As}_4\text{V}$  is:

```
sprocess> pdbGet Si KMC As Etot.Complex As4V  
-5.4
```

The barriers are not defined by default:

```
sprocess> pdbGet Si KMC F EbarrierIV.Complex  
sprocess> pdbGet Si KMC F EbarrierDopant.Complex
```

The charge value for the clusters is retrieved with:

```
sprocess> pdbGet Si KMC F e0.Complex  
sprocess> pdbGet Si KMC B e0.Complex  
B3 0 B3I 0 B3I2 0 B3I3 0  
B2 0 B2I 0 B2I2 0 B2I3 0  
BI2 0
```

No value means that they are neutral.

**NOTE** The impurity cluster model and the activation or deactivation of clusters can be calibrated further fitting the potential energies. For further accuracy, Advanced Calibration also can be used.

When a particular energy for a particular configuration is not specified (that is, when input in the parameter file exists for an  $\text{A}_n\text{I}_m$  or  $\text{A}_n\text{V}_m$  impurity cluster), Sentaurus Process KMC assumes this configuration to be unstable. When a barrier energy is not specified, a value of 0 eV (no barrier) is assigned.

All impurities are allowed to form impurity clusters with  $I$ ,  $V$ , or both. If an impurity does not form impurity clusters, the default can be changed, modifying the parameters and the interactions (see [Interactions of Impurity Cluster Model on page 485](#)).

## Emission

Impurity clusters can emit both neutral interstitials (vacancies) or mobile dopants:



Sentaurus Process KMC computes the emission frequencies as:

$$v_{emission} = v_{0, emission} \times \exp\left(-\frac{E_{emission}}{k_B T}\right) \quad (742)$$

The emission energies are:

$$E_{emission}(I) = E_m(I) + E_{barrier}(A_n I_m) + \max(0, E^{AnIm}_b(I)) \quad (743)$$

$$E_{emission}(A_i) = E_m(A_i) + E_{barrier}(A_n I_m) + \max(0, E^{AnIm}_b(A_i)) \quad (744)$$

$E_m$  is the migration energy of the emitted species, and both  $E^{AnIm}_b(I)$  and  $E^{AnIm}_b(A_i)$  have been shown above. The emission prefactors for dopant and I or V emission depend on the model used.

When `UseCaptVol.Complex` is set to `true`, the emission prefactors are proportional to the capture volumes of the impurity clusters:

- $v_{0, emission}(A_i) = K(A_i) V_{capt}(A_n I_m)$
- $v_{0, emission}(I) = K(I) V_{capt}(A_n I_m)$

$V_{capt}(A_n I_m)$  is the capture volume for each impurity cluster, defined in the PDB as `CaptVol.Complex`, and the constant  $K$  is a parameter named `D0.Cluster` in the PDB.

**NOTE** The unit of the capture volumes is the capture volume of one point defect.

If `UseCaptVol.Complex` is set to `false`, Sentaurus Process KMC uses the default old model, in which the capture volumes are internally fixed to be  $m$  for  $I$  emission and  $\min(n, m)$  for  $A_i$  emission. The use of this default model is not suggested, since it does not lead to microscopic reversibility.

When a particle is emitted, the impurity cluster tests whether the number of remaining particles is enough to maintain the cluster. If there is only an interstitial (vacancy) or an interstitial and a dopant, the cluster dissolves leaving an interstitial or a mobile paired dopant, respectively.

## Parameters

The prefactor constants are:

```
sprocess> pdbGet Si KMC As D0.Cluster  
As,AsV 2.1  
As,V 10  
sprocess> pdbGet Si KMC B D0.Cluster  
B,Bi 3  
B,I 150
```

The notation for these prefactors is as follows: Two strings are needed, separated by a comma. The second string represents the emitted particle for which the parameter is being defined. The first string represents the type of cluster, and it is needed to define a different prefactor for emitting a  $B_i$  from a B cluster rather than from a hypothetical BF cluster. For example, the emission of  $B_i$  from  $B_2I_2$  will use B,Bi, while from  $B_2F_3I_2$ , it will use BF,Bi. This last one can be defined in KMC Si B and KMC Si F, but if defined in both of them with different values, it will generate an error.

The capture volume parameters are:

```
sprocess> pdbGet KMC UseCaptVol.Complex  
0  
sprocess> pdbGet Si KMC B CaptVol.Complex  
B3 1 B3I 1 B3I2 2 B3I3 3  
B2 1 B2I 1 B2I2 2 B2I3 2  
B2I2 1
```

The notation for capture volumes is as following: If only the cluster is specified, that applies to all emissions for that particular size. If a cluster size and a particular particle are specified, separated by a comma, that applies to that cluster emitting only that particle. For example, the following applies only to emission if I by  $B_2I_2$ :

```
pdbSet Si KMC B CaptVol.Complex B2I2,I 6
```

The rest of the parameters needed for emission are the same as in [Growth of Impurity Clusters on page 473](#).

---

## Recombination

Impurity clusters can trap incoming neutral Vs ( $I_s$ ) and recombine them with internal Is (Vs):



The capture probability is:

$$P_{capture} = \exp\left(-\frac{E_{capture}}{k_B T}\right) \quad (746)$$

The associated energies are:

$$E^{AnIm}_{capture} = E^{AnIm}_b - E_{pot}(V) - E_{pot}(I) \quad (747)$$

and:

$$E^{AnIm}_b = E(A_n I_{m-1}) - E(A_n I_m) \quad (748)$$

After the *IV* pair recombination, the cluster size is tested and, if necessary, it is dissolved as previously explained.

The parameters used for recombination of point defects are the same as in [Growth of Impurity Clusters on page 473](#).

## Frank–Turnbull Mechanism

A generalized Frank–Turnbull (FT) mechanism is the emission of a neutral *V* (*I*) from an  $A_n I_m$  ( $A_n V_m$ ) impurity cluster by the formation of a Frenkel pair (*IV*):



or:



Sentaurus Process KMC includes the FT mechanism to maintain microscopic reversibility. Since impurity clusters recombine incoming *Is* or *Vs*, the opposite mechanism (FT) also is needed. Usually, this mechanism is unfavorable, but for some particular configurations, the energetic differences between them can enable the formation of *IV* pairs and, therefore, the emission of particles using the FT mechanism (see [Figure 55 on page 480](#)).

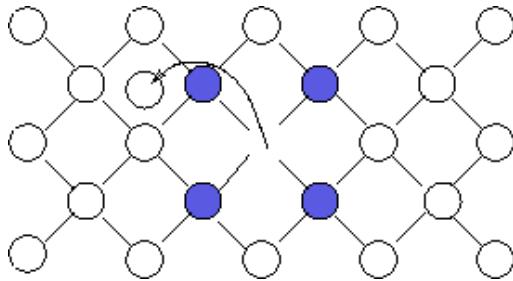


Figure 55 Example of FT mechanism: an  $\text{As}_4$  cluster can emit an interstitial to become an  $\text{As}_4\text{V}$  impurity cluster: blue is arsenic and white is silicon

The vacancy (interstitial) emission frequency is computed as:

$$v_{emission} = v_{0, emission} \times \exp\left(-\frac{E_{emission}}{k_B T}\right) \quad (751)$$

being:

$$E_{emission}(V) = E_m(V) + \max(0, E^{AnIm}_b(V)) \quad (752)$$

and:

$$E^{AnIm}_b(V) = E_{pot}(I) + E_{pot}(V) + E_{pot}(A_n I_{m+1}) - E_{pot}(A_n I_m) \quad (753)$$

where the potential energies for the clusters and the point defects include pressure and Ge corrections.

## Parameters

The parameters used are the same as in [Growth of Impurity Clusters on page 473](#). The potential energies for interstitial and vacancies are specified for the material as Ef:

```
sprocess> pdbGet Si KMC I Ef
4.0
sprocess> pdbGet Si KMC V Ef
3.8
```

The corrections to the potential energies for I and V are VF and Alloy.Ef for pressure and Ge, respectively:

```
sprocess> pdbGet Si KMC I Alloy.Ef
I 0.0
sprocess> pdbGet Si KMC I VF
I 0.0
```

The prefactor for I and V emission is computed automatically for impurity clusters with only one dopant (for example,  $B_nI_m$  or  $As_nV_m$  clusters) and must be specified for other cases. For example, in a case with  $AsPV$  clusters, the prefactors for Frank–Turnbull emission are specified as follows:

```
pdbSet Si KMC As D0.Cluster AsP,V 50
pdbSet Si KMC As D0.Cluster AsP,I 50
```

The following is also valid:

```
pdbSet Si KMC P D0.Cluster AsP,V 50
pdbSet Si KMC P D0.Cluster AsP,I 50
```

## Complementary Recombination

Some impurities diffuse using both interstitial and vacancy mechanisms. For these cases, the impurity clusters can react with both of them. For example, an  $A_nV_m$  impurity cluster can grow trapping  $AsV$ , as previously explained, and can interact with an incoming  $As_i$ , trapping the  $As$  and recombining the  $I$  with one internal vacancy. This implies to take into account the reaction:



These complementary recombinations of neutral particles are allowed with a probability of:

$$P_{capture} = \begin{cases} \exp(-E_{capture}/(k_B T)) & E_{capture} > 0 \\ 1 & E_{capture} \leq 0 \end{cases} \quad (755)$$

The capture energies are computed as:

$$E_{capture} = \begin{cases} E_{pot}(A_{n+1}V_{m-1}) - E_{pot}(A_nV_m) - E_f(V) - E_f(I) - E_{pot}(A_i) & m > 0 \\ E_{pot}(A_{n+1}V_m) - E_{pot}(A_nV_m) - E_{pot}(A_i) + E_m(I) - E_m(A_i) & m \equiv 0, n > 1 \\ E(A_i \rightarrow A) & m \equiv 0, n \equiv 1 \end{cases} \quad (756)$$

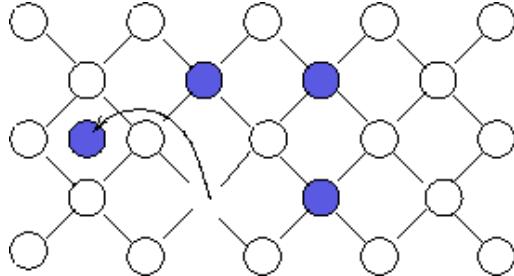
where  $E(A_i \rightarrow A)$  is an internal parameter that cannot be changed.

## Parameters

The parameters used are the same as in [Frank–Turnbull Mechanism on page 479](#). The potential energy for the paired dopant is the binding energy of the pair corrected with the Fermi-level dependency.

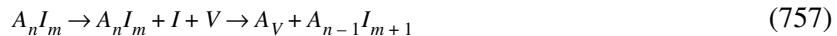
## Complementary Emission

To maintain microscopic reversibility, the reverse reaction to complementary recombination must be defined (see [Figure 56](#)).



**Figure 56** Example of complementary emission: the cluster emits an interstitial that takes an impurity and generates a vacancy; blue is arsenic and white is silicon

The equation for this process is:



Its emission frequency is computed using the emission frequency equation:

$$E_{emission} = E_m(A_V) + \max(0, E^{AnIm}_b(A_V)) \quad (758)$$

where:

$$E^{AnIm}_b(A_V) = E_f(I) + E_f(V) + E_{pot}(A_{n-1}V_{m+1}) - E_{pot}(A_nI_m) \quad (759)$$

## Parameters

The parameters used are the same as in [Recombination on page 478](#).

For simple impurity clusters, those with only one impurity ( $B_n I_m$ ,  $As_n V_m$ , and so on), the prefactor for emission is calculated automatically. For complex impurity clusters, (such as  $As_n P_o V_m$ ), the prefactor must be written explicitly:

```
pdbSet Si KMC As D0.Cluster AsP,Asi 50
```

## Charge Dependency

### Neutral Reactions

In previous discussions, all the impurity clusters are assumed to be neutral and, consequently, there are no explicit charge Fermi-level dependencies. Nevertheless, there are nonexplicit dependencies. In particular, for clusters emitting impurity-paired dopants, the emission energy depends on the binding of the paired dopants, which, in turn, contains a Fermi-level dependency.

The Fermi-level dependency of the binding energy is related to the level of the neutral-paired dopant in the band gap. This level also depends on the temperature and the bandgap narrowing.

All the previous dependencies are included by default, except the indirect dependency on the bandgap narrowing, which can be switched off and on using:

```
pdbSet <material> KMC BandGap Correct.Complex <true | false>
```

### Nonneutral Reactions

Assume the following reaction:



The potential energy for  $B_n I_m^a$  is defined with respect to a ground state that produces the impurity cluster in a neutral reaction. This means that:

$$nB^- + mV^0 + \begin{cases} -(a+n)e^- \Rightarrow a+n < 0 \\ (a+n)h^+ \Rightarrow a+n > 0 \end{cases} \quad (761)$$

is the ground state for  $As_n V_m^a$ . Consequently, an account of holes and electrons must be followed during the reaction. In particular, calling the initial cluster  $i$  and the final one  $f$ , these accounts are:

- $h_i^+ = \begin{cases} a+n \Rightarrow a+n > 0 \\ 0 \Rightarrow a+n < 0 \end{cases}$  ,  $e_i^- = \begin{cases} 0 \Rightarrow a+n > 0 \\ -a-n \Rightarrow a+n < 0 \end{cases}$
- $h_{f1}^+ = \begin{cases} b+o \Rightarrow n+o < 0 \\ 0 \Rightarrow b+a < o \end{cases}$  ,  $e_{f1}^- = \begin{cases} 0 \Rightarrow b+o > 0 \\ -b-o \Rightarrow b+o < 0 \end{cases}$

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Impurity Clusters

The final state must account for the charge in the emitted particle. Calling  $d$  the charge of the substitutional dopant of the emitted species  $X$  (in other words,  $d = -1$  if  $X^c = B_i^c$  or  $d = 0$  if  $X^c = I^c$ ), the final accounts for holes and electrons are:

- $h_f^+ = h_{f1}^+ + \begin{cases} c-d \Rightarrow c-d > 0 \\ 0 \Rightarrow c-d < 0 \end{cases}$

- $e_f^- = e_{f1}^- + \begin{cases} 0 \Rightarrow c-d > 0 \\ d-c \Rightarrow c-d < 0 \end{cases}$

This allows writing the first energetic term for the binding energy as:

$$E_{\text{charges}} = (e_i^- - e_f^-)(E_g - e_F) + (h_i^+ - h_f^+)e_F \quad (762)$$

The second term is the obvious difference in potential energies:

$$E_{\text{clusters}} = E_{\text{pot}}(B_n I_m) - E_{\text{pot}}(B_o I_p) \quad (763)$$

The binding energy of the emitted particle is also needed, including the transition from the *neutral* state  $d$  to the current emitted state:

$$E_b(X^c) = E_b(X^d) + E \left( X^d + \begin{cases} (d-c)e^- \Rightarrow d-c > 0 \rightarrow X^c \\ (c-d)h^+ \Rightarrow c-d > 0 \end{cases} \right) \quad (764)$$

In addition, only in cases where a Frank–Turnbull emission is involved ( $X^c = V^c$  or  $X^c = BV^c$ ), the pair recombination energy is:

$$E_{\text{recom}} = E_f(I) + E_f(V) \quad (765)$$

This gives a binding energy of:

$$E^{B_n I_m b}(X^c) = -E_{\text{charges}} - E_{\text{clusters}} - E_b(X^c) + E_{\text{recom}} \quad (766)$$

That finally allows computing the emission energy:

$$E_{\text{emission}}(X^c) = E_m(X^c) + E_{\text{barrier}}(B_n I_m) + \max(0, E^{B_n I_m b}(X^c)) \quad (767)$$

**NOTE** All the previous energies (such as potential, binding, and migration) are computed including hydrostatic pressure, SiGe, and bandgap narrowing local corrections.

## Interactions of Impurity Cluster Model

You can modify all the interactions involved in the impurity cluster model. The impurity clusters can be enabled or disabled with the Boolean parameter `Implement.Complex`. For example, to disable the  $F_n V_m$  impurity clusters, use:

```
pdbSet Si KMC F Implement.Complex 0
```

When the impurity clusters are enabled, you can set and unset the particular reactions using the `ReactionsCluster` parameter:

```
pdbSet Si KMC <dopant> ReactionsCluster <reaction> <true | false>
```

where `reaction` is a string with two fields, separated by a comma. The first field is the name of the impurity cluster, and the second is the name of the reacting particle. Spaces are not allowed between these fields. The setting or unsetting of these reactions enables or disables the specified reactions and its reverse ones. This is performed to maintain the microscopic reversibility. For example, to disable the capture of a vacancy by  $As_2$  to growth to  $As_2V$ :

```
pdbSet Si KMC As ReactionsCluster As2,V false
```

This also disables the inverse reaction, in other words, the emission of  $V$  by  $As_2V$ . To enable the recombination of  $I$  by an  $As_4V$  cluster:

```
pdbSet Si KMC As ReactionsCluster As4V,I true
```

This reaction also enables the FT emission of  $I$  by  $As_4$ , that is,  $As_4 \rightarrow As_4V + I$ .

Enabling a reaction does not mean that the reaction will happen; it depends on the energetics. If the reaction is unfavorable, it will not occur (but the inverse will). Disabling a reaction will forbid the reaction to occur, even if it is described by the parameters as favorable. Any reaction not listed in `ReactionsClusters` is disabled.

## Complex Impurity Clusters

To enable impurity clusters with more than one dopant (for example, an  $As_2PV$ ), the switches for both the `As` and `P` clusters should be on:

```
pdbSetBoolean Si KMC As Implement.Complex 1
pdbSetBoolean Si KMC P Implement.Complex 1
```

To enable the cluster reaction  $As_2 + PV \leftrightarrow As_2PV$  (assuming  $As_2$  is predefined), use the `As` or the `P` to define the reaction. If both are used with different values, an error message will be displayed. In this example, they are defined in `As`:

```
pdbSet Si KMC As ReactionsCluster As2,PV true
```

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The energy and capture volume of this new cluster must be defined as usual:

```
pdbSet Si KMC P Etotal.Complex PAs2V -3.0  
pdbSet Si KMC P CaptVol.Complex PAs2V 1.3
```

The I, V, and PV emission prefactors are:

```
pdbSet Si KMC P D0.Cluster PAs,I 0.5  
pdbSet Si KMC P D0.Cluster PAs,V 0.5  
pdbSet Si KMC P D0.Cluster PAs,PV 0.1
```

Finally, for AsV emission from the cluster As<sub>2</sub>PV, allow the reaction AsP + AsV  $\leftrightarrow$  As<sub>2</sub>PV by defining:

```
pdbSet Si KMC P ReactionsClusters PAs,AsV true
```

This also enables the formation of the clusters through the reaction of these particles.

## Parameters

To show the parameters involved in the impurity cluster reactions, arsenic is used as an example. AsV clusters are allowed:

```
sprocess> pdbGet Si KMC As Implement.Complex  
1
```

Since AsV clusters are allowed in the Sentaurus Process KMC simulation, they require some enabled reactions. The reactions are explained in [Percolation on page 475](#) and allow deactivation without arsenic diffusion:

```
sprocess> pdbGet Si KMC As ReactionsCluster  
As2,As true  
As3,As true
```

Reactions to grow capturing V and to shrink emitting them are:

```
As2,V true  
As3,V true  
As4,V true
```

Capture or emission of AsV is:

```
As2,AsV true  
As3,AsV true
```

Recombination of interstitials and Frank–Turnbull emission of interstitials are:

```
As2V, I    true
As3V, I    true
As4V, I    true
```

Recombination of interstitials, capture of arsenic, and emission of As<sub>i</sub> are:

```
As2V,Asi   true
As3V,Asi   true
```

The following rules must be satisfied to allow a reaction between a particle and an impurity cluster:

- The first field must be a correct impurity cluster, and the second must be a defined particle.
- The particle must be an interstitial or a vacancy of a paired dopant. The resulting cluster must be defined (in Etot<sub>al</sub>.Complex and CaptVol.Complex).
- Only nonrepulsive interactions are allowed, except for percolation. The reactions do not need to conserve the charge.

Impurity clusters require an initial impurity cluster or ‘seed’ to begin the ripening. This initial cluster is formed with the reactions of two particles. These reactions are explained in [Enabling and Disabling Interactions on page 418](#).

## Setting Up Impurity Clusters in a Material

To set up an impurity cluster in a material (for example, B<sub>n</sub> in amorphous silicon), the following PDB parameters must be created:

- First, the cluster must be allowed:

```
pdbSetBoolean aSi KMC B Implement.Complex true
```

- Second, an emission prefactor for the cluster, cluster potential energies, barriers, capture volumes, and stress corrections must be defined:

```
pdbSetDoubleArray aSi KMC B D0.Cluster      { B 3.0 }
pdbSetDoubleArray aSi KMC B Etotal.Complex { B2 -0.45 B3 -2.5 }
pdbSetDoubleArray aSi KMC B EbarrierDopant.Complex { }
pdbSetDoubleArray aSi KMC B CaptVol.Complex { B2 1.5 B3 2.0 }
pdbSetDoubleArray aSi KMC B VF.Complex      { }
```

- Third, for these clusters to form, you must introduce a reaction path:

```
pdbSetArray aSi KMC B ReactionsPointDefect { B,B true }
pdbSetArray aSi KMC B ReactionsCluster     { B2,B true }
```

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Fermi-Level Effects: Charge Model

- None of this will happen without a mobile particle allowing for growing and emission:

```
pdbSet aSi KMC B Dm B 3.0e-3  
pdbSet asi KMC B Em B 2.1
```

**NOTE** The impurity cluster parameters (energies, barriers, capture volumes, stress corrections) must be specified in the PDB only when the cluster is implemented (with `Implement.Complex true`). This saves many parameters in the description of impurities without impurity clusters.

---

## Fermi-Level Effects: Charge Model

Point defects (*I*, *V*) and impurity atoms (B, As) can appear in different charge states in silicon, while extended defects and impurity clusters have a fixed charge state in Sentaurus Process KMC. Impurity atoms are neutral in materials using the simple model.

For example, interstitials and vacancies can be triple negative, double negative, double positive, triple positive, neutral, positive, or negative. Some species and charge states are listed in [Table 61](#). You can customize these definitions. The maximum charge state for point defects is  $\pm 3$  and, for impurity paired defects, it is  $\pm 2$ .

Table 61 Species and charge states used in Sentaurus Process KMC

Species	Charge states
I	$I^{+++}$ , $I^{++}$ , $I^+$ , $I^0$ , $I^-$ , $I^{--}$ IPPP, IPP, IP, I, IM, IMM, IMMM
V	$V^{+++}$ , $V^{++}$ , $V^+$ , $V^0$ , $V^-$ , $V^{--}$ VPPP, VPP, VP, V, VM, VMM, VMMM
As	$As^+$ , $As_i^+$ , $As_i^0$ , $AsV^+$ , $AsV^0$ , $AsV^-$ As, AsiP, Asi, AsVP, AsV, AsVM
B	$B^-$ , $B_i^+$ , $B_i^0$ , $B_i^-$ B, BiP, Bi, BiM
C	$C^0$ , $C_i^0$ C, Ci
F	$F^0$ , $Fl^0$ , $FV^0$ F, Fl, FV
Sb	$Sb^+$ , $Sb_i^0$ , $Sb_i^+$ , $SbV^-$ , $SbV^0$ , $SbV^+$ Sb, Sbi, SbiP, SbVM, SbV, SbVP

Table 61 Species and charge states used in Sentaurus Process KMC

Species	Charge states
In	$\text{In}^-$ , $\text{In}_i^0$ , $\text{In}_i^-$ , $\text{InV}^0$ , $\text{InV}^-$ $\text{In}$ , $\text{In}_i$ , $\text{IniM}$ , $\text{InV}$ , $\text{InVM}$
P	$\text{P}^+$ , $\text{P}_i^0$ , $\text{P}_i^+$ , $\text{PV}^0$ , $\text{PV}^-$ , $\text{PV}^+$ $\text{P}$ , $\text{Pi}$ , $\text{PiP}$ , $\text{PV}$ , $\text{PVM}$ , $\text{PVP}$

Charge states can be modeled using different approaches. The most intuitive approach is to add a charge ‘label’ to each particle. Nevertheless, because the migration energy (and maybe some other parameters) change with the charge state, each of these states requires a full set of parameters.

## Sentaurus Process KMC Approach

No charge label is defined for particles. The charge is implicitly assumed in each particular particle, and there are different particles for each charge state. This implies the necessity of defining the interactions one by one, according not only with the particle type, but also with its charge state.

The charge is represented in a quasiamstomistic approach to account for the fact that electron transport is several orders of magnitude faster than atomic transport. The charge magnitudes (for example, Fermi level and bandgap width) are associated with each internal box in the simulation. Consequently, there can be local changes between different boxes, but the charge magnitudes are considered to be homogenous in each Sentaurus Process KMC internal element.

## Assumptions

Sentaurus Process KMC takes the energy reference in the valence band. The following assumptions also are taken:

- Charge reactions are faster than structural reactions [46]. Consequently, charges are updated instantaneously.
- The formation energy for neutral species (for example,  $E_f(\text{I}^0)$ ) is not dependent on the Fermi level. Sentaurus Process KMC takes the formation energies for neutral species as parameters using them to compute the energies for nonneutral species.
- Potential energies for impurity clusters are not dependent on the Fermi level. For example, Sentaurus Process KMC defines the potential energy for  $\text{As}_n V_m^a$  as the energy returned by the system in the reaction  $n\text{As}^+ + m\text{V}^0 + (n-a)e^- \rightarrow \text{As}_n V_m^a$  (assuming that  $n - a > 0$  ).

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Fermi-Level Effects: Charge Model

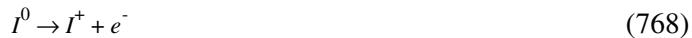
- The electronic level dependency with temperature is proportional to the bandgap temperature dependency. The same applies to bandgap narrowing. This assumption allows Sentaurus Process KMC to establish proportionality relations to compute the electronic levels and bandgap narrowing at different temperatures using a known value for one particular temperature.
- Substitutional dopants are always ionized; that is, substitutional boron is always  $B^-$  and substitutional arsenic is always  $As^+$ .
- The properties inside each Sentaurus Process KMC element are constant. Properties can change between internal elements.

For further references on similar KMC charge models, see [1][47][48].

---

## Formation Energies for Charged Species

Taking  $I^+$  as an example, in the reaction:



the energy needed to take an electron from an  $I^0$  and obtain  $I^+ + e^-$  is denoted as  $e(+,0)$ , and is measured from the valence band. The formation energy for a positive interstitial is:

$$E_f(I^+) = E_f(I^0) + e_F - e(+,0) \quad (769)$$

where  $e_F$  is the Fermi level. Consequently, the concentration between different interstitial charge species using as a reference the neutral concentration is:

$$\frac{[I^0]}{[I^+]} = \exp\left(\frac{e_F - e(+,0)}{k_B T}\right) \quad (770)$$

$$\frac{[I^+]}{[I^0]} = \exp\left(\frac{e_F - e(0, -)}{k_B T}\right) \quad (771)$$

The electronic levels (for  $T = 0$  K) are specified in the parameter database as  $e0$ . They are defined only for silicon. They can be changed with:

```
pdbSet Si KMC <I | V | impurity> e0 <species> <n>
```

for example:

```
pdbSet Si KMC I e0 IP 0.35
```

## Parameters

The bandgap levels for interstitials and vacancies can be retrieved with:

```
sprocess> pdbGet Si KMC I e0
IM 1.0
IP 0.35
sprocess> pdbGet Si KMC V e0
VMM 1.06
VM 0.6
VP 0.03
VPP 0.13
```

They also are specified for dopants, like As:

```
sprocess> pdbGet Si KMC As e0
AsVM 0.77
AsVP 0.3
AsiP 0.1
```

**NOTE** The modification of these parameters affects both extrinsic and intrinsic diffusion.

## Binding Energies for Particles

The binding energy needed for pairing and breakup reactions is only specified for the reaction with the neutral interstitial or vacancy. For example, for boron, the binding energy is specified for the reaction  $B^- + I^0 = B_i^-$ . The other binding energies (for example,  $B^- + I^+ = B_i^0$ ) are computed using the binding energy for the above reaction and the energy levels associated to the charge transitions [48]:

$$E_b(B_i^0) = E_b(B_i^-) + e(B_i)(0, -) - e(I)(+, 0) \quad (772)$$

The activation energy for the  $B_i^0$  breakup is  $E_b(B_i^0) + E_m(I^+)$ . Because electronic levels scale with  $E_g$  (as shown below), a slight dependency with  $T$  is introduced in these calculated binding energies.

## Binding Energies for Impurity Clusters

For an example of how to compute the binding energy for an impurity cluster, see [Nonneutral Reactions on page 483](#).

---

## Temperature Dependency

The bandgap width used in Sentaurus Process KMC is given by the expression [49]:

$$E_g(T) = E_g(T=0) - \frac{AT^2}{B+T} \quad (773)$$

Using the assumption of proportionality with the band gap, Sentaurus Process KMC assumes that the electronic levels at different temperatures can be computed as:

$$e(j+1,j)(T) = e(j+1,j)(0) \times \frac{E_g(T)}{E_g(0)} \quad (774)$$

Effective state density of conduction and valence bands follows similar expressions:

$$N_c(T) = N_c(300) \times \left(\frac{T}{300}\right)^{\exp N_c} \quad (775)$$

$$N_v(T) = N_v(300) \times \left(\frac{T}{300}\right)^{\exp N_v} \quad (776)$$

Finally, Sentaurus Process KMC uses the values to compute the intrinsic levels and intrinsic carrier densities:

$$e_i(T) = \frac{E_g(T)}{2} + \left(\frac{k_B T}{2}\right) \ln\left(\frac{N_v}{N_c}\right) \quad (777)$$

$$n_i(T) = \sqrt{N_c N_v} \times \exp\left(-\frac{E_g(T)}{2k_B T}\right) \quad (778)$$

## Parameters

The required parameters are specified in the parameter database under the BandGap folder:

Eg0	Bandgap width at 0 K ( $E_g(0)$ ).
Agap	Bandgap width temperature dependency parameter ( $A$ ).
Bgap	Bandgap width temperature dependency parameter ( $B$ ).
Nc300	Effective state density for the conduction band, at 300 K ( $N_c(300)$ ).
Nv300	Effective state density for the valence band, at 300 K ( $N_v(300)$ ).

expNc      Effective state density temperature dependency parameter (conduction).

expNv      Effective state density temperature dependency parameter (valence).

They can be changed using `pdbSet`. For example, to set the bandgap width at 0 K, use:

```
pdbSet Si KMC BandGap Eg0 1.17
```

The parameters for the bandgap temperature dependency are defined for silicon in the `BandGap` folder:

```
sprocess> pdbGet Si KMC BandGap Eg0
1.17
sprocess> pdbGet Si KMC BandGap Agap
0.000473
sprocess> pdbGet Si KMC BandGap Bgap
636.0
sprocess> pdbGet Si KMC BandGap Nc300
3.2e+19
sprocess> pdbGet Si KMC BandGap Nv300
1.8e+19
sprocess> pdbGet Si KMC BandGap expNc
1.5
sprocess> pdbGet Si KMC BandGap expNv
1.5
```

---

## Charge Attractions and Repulsions

The short-range repulsions between charged particles have been implemented forbidding interactions between particles in the same charge state (except for percolation reactions; see [Percolation on page 475](#)). Long-range forces are considered automatically due to the bias induced in the particle migration by the local Fermi level.

---

## Fermi-Level Computation

Sentaurus Process KMC computes the Fermi level assuming charge neutrality and Fermi-Dirac statistics. It simply makes the number of charges in each cell element equal to the concentration of substitutional dopants and charged impurity clusters in the box. The presence of mobile charged particles is neglected.

The charge concentration for each element is an average of the charge concentration in the neighborhood. The averaging radius is taken as the parameter `Smooth.Radius`. The power of

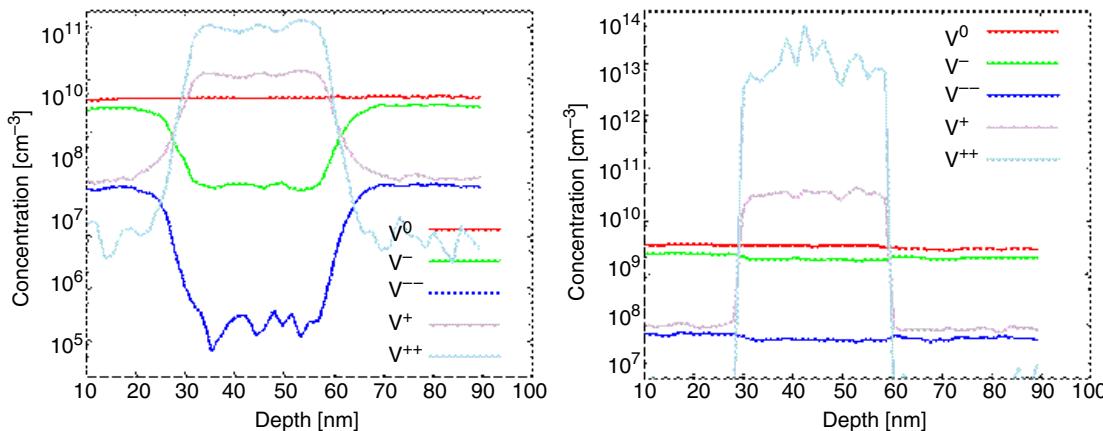
## 5: Atomistic Kinetic Monte Carlo Diffusion

### Fermi-Level Effects: Charge Model

this average is controlled with the parameter `Smooth.Power`. This average is important because of the atomistic nature of the simulation.

Without this averaging, a medium-dose doped sample, with some elements filled up with particles and some empty ones, could be considered as a set of intrinsic (empty) boxes and a few boxes with a very high concentration.

For example, a dopant concentration of  $1 \times 10^{20} \text{ cm}^{-3}$  corresponds to one particle in  $10 \text{ nm}^3$ . The volume of an internal element may be as small as  $1 \text{ nm}^3$ . This means one particle per 10 boxes. Without any charge averaging, a moving interstitial would diffuse intrinsically in nine empty boxes and extrinsically in one box. With the average, the interstitial ‘sees’ the right concentration of  $1 \times 10^{20} \text{ cm}^{-3}$  and diffuses according to this concentration (see [Figure 57](#)).



**Figure 57** Simulated vacancy profiles for a p-sample (from 30 to 60 nm) for different vacancy charge states: (*left*) smoothing out the charge concentration and (*right*) incorrect results without smoothing

## Parameters

This smoothing is a default Sentaurus Process KMC feature performed by an ultrafast algorithm and is controlled only by the cutoff radius (in nanometers) specified in the parameter database:

```
sprocess> pdbGet Si KMC BandGap Smooth.Radius  
7
```

**NOTE** To switch off this local computation and to set up a constant, user-defined dopant concentration, experienced users may want to use the following command, where <dopant concentration> is a positive quantity for n-type devices and a negative one for p-type devices:

```
pdbSetDouble KMC setDopantConc <dopant concentration>
```

## Updating Charge States

The charge model of Sentaurus Process KMC assumes that the electronic transport and reactions are faster than the atomic transport and reactions. Therefore, it is necessary to implement mechanisms to update the charge distribution (and the local Fermi level) that follows the structural changes. Since the equilibrium ratios depend only on the Fermi level, it is necessary to update them each time the Fermi level varies.

There are two reasons for local changes in the Fermi level:

- Mobile particles diffuse between elements with different Fermi levels.
- The electronic concentration in one element changes.

Besides, each time a new particle appears or disappears because of pairing or breakup reactions, it is necessary to ensure that the charge state of the new particle is consistent with its local Fermi level.

Different mechanisms are implemented to maintain the correct charge ratios. All are performed at the same time, but they apply to different scenarios.

## Electronic Concentrations and Charge-State Ratios

An update algorithm periodically reviews all the particles and updates the Fermi level and the proportions of charged particles in each element. The algorithm:

- Smooths the charge distribution.
- Computes the Fermi level for each box using the charge neutrality assumption.
- Establishes the appropriate charge ratios.

**NOTE** This update algorithm slows down the simulation. It is crucial to follow the changes in the Fermi level, but without spending too much CPU time.

## Mobile Particles

Mobile particles see different Fermi levels when they move from one element to another. Therefore, the charge of a mobile particle needs to be updated each time it crosses the boundaries between boxes. At the same time, particles change their charge state to maintain the proper charge distribution; consequently, they need extra updates. This is implemented with an algorithm that updates the charge of mobile particles each time they perform a migration jump. This algorithm also considers the migration frequency of each particle, as explained in [48], to avoid artificial concentration increases in the slow diffusing species concentration.

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Fermi-Level Effects: Charge Model

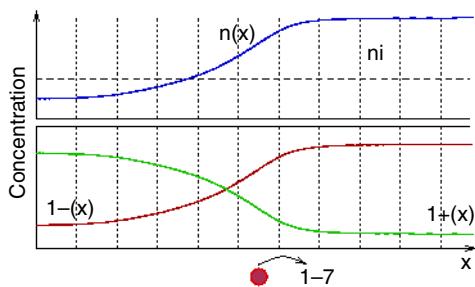


Figure 58 A mobile particle ( $I^-$ ) sees different electronic properties when jumping from one element to a different one. Its charge state must be updated to reproduce the expected macroscopic concentration.

## Pairing and Breakup Reactions

After pairing or breakup reactions, some species appear and disappear in the Sentaurus Process KMC elements. To ensure that the concentration of these species maintains the correct proportions, a breakup, pairing charge update mechanism is implemented. It computes the probability of the new particles to be in a particular charge state.

### Parameters

The charge update algorithm uses only the `ChargeVarPercent` parameter in the parameter database, and it accounts for the maximum relative error allowed for the Fermi-level updates. This parameter is a compromise between accuracy and efficiency.

Decreasing its value leads to more accurate but slower simulations, and the charge model can overload your computer resources.

Increasing its value speeds up the simulation at the cost of accuracy:

```
sprocess> pdbGet KMC ChargeVarPercent  
0.25
```

**NOTE** Only small modifications to `ChargeVarPercent` are recommended.

In addition, you can force charge updates during each implantation step at certain dose levels, or you can force a certain number of charge updates. To force such charge updates, you can define either of the following parameters:

```
pdbSet KMC MCImplant.Charge.Update.Dose <n>  
pdbSet KMC MCImplant.Charge.Updates <n>
```

Using these parameters does not disable automatic charge updates. The default value for MCImplant.Charge.Update.Dose is 1e18 and that for MCImplant.Charge.Updates is 0. If both parameters are defined, the parameter specifying the higher number of charge updates is used.

**NOTE** Do not use a very small value for MCImplant.Charge.Update.Dose to force frequent charge updates, as it can slow down performance significantly.

## Electric Drift

The charge model of Sentaurus Process KMC considers the:

- Introduction of an electric field, related to the local charge variations.
- Existence of forces acting over the charged species; these forces generate a bias in the diffusion – the *electric drift*.

Sentaurus Process KMC models electric bias modifying the jump probabilities to account for the space anisotropy produced when an electric field is present.

A particle inside the electric field can jump in both directions, but the probability of jumping following the electric field is higher. Consequently, a ‘migration barrier’ is implemented. The barriers are related to the relative concentration of each species. For example, for an I<sup>+</sup> jumping from a position  $x_2$  in a box to a position  $x_1$  in a different box, if  $P(x_2) > P(x_1)$ , where  $P$  is the probability of an interstitial having a positive charge, the jump is always possible. Otherwise, there is a probability of  $1 - [P(x_2)]/[P(x_1)]$  of being rejected.

For an I<sup>+</sup> particle, the jump is accepted with a probability of:

$$\frac{P(x_2)}{P(x_1)} = \exp\left(\frac{[e_F - e(+,0)]_2 - [e_F - e(+,0)]_1}{k_B T}\right) \quad (779)$$

where typically, if there are no bandgap narrowing effects,  $e(+, 0)_2 = e(+, 0)_1$  and:

$$\frac{P(x_2)}{P(x_1)} = \exp\left(\frac{e_{F2} - e_{F1}}{k_B T}\right) \quad (780)$$

The subscripts 1 and 2 refer to magnitudes in different elements. [Figure 59 on page 498](#) shows an energy diagram of this process. The number of rejected jumps for each axis is shown in a report at the end of the annealing.

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Fermi-Level Effects: Charge Model

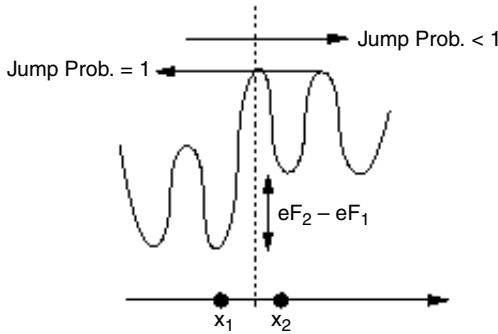


Figure 59 Energy diagram showing the jump process

## Bandgap Narrowing

### Narrowing due to Dopant Concentration

Sentaurus Process KMC includes doping-induced energy shifts of the conduction band minimum and the valence band maximum. The narrowing of the fundamental band gap is presented as the function [50] for n-type semiconductors:

$$\Delta E_{gdc} = A_{cn1/4} \left( \frac{N^+}{10^{18}} \right)^{1/4} + A_{cn1/3} \left( \frac{N^+}{10^{18}} \right)^{1/3} + A_{cn1/2} \left( \frac{N^+}{10^{18}} \right)^{1/2} \quad (781)$$

$$\Delta E_{gdv} = A_{vn1/4} \left( \frac{N^+}{10^{18}} \right)^{1/4} + A_{vn1/3} \left( \frac{N^+}{10^{18}} \right)^{1/3} + A_{vn1/2} \left( \frac{N^+}{10^{18}} \right)^{1/2} \quad (782)$$

and for p-type semiconductors:

$$\Delta E_{gdc} = A_{cp1/4} \left( \frac{N^-}{10^{18}} \right)^{1/4} + A_{cp1/3} \left( \frac{N^-}{10^{18}} \right)^{1/3} + A_{cp1/2} \left( \frac{N^-}{10^{18}} \right)^{1/2} \quad (783)$$

$$\Delta E_{gdv} = A_{vp1/4} \left( \frac{N^-}{10^{18}} \right)^{1/4} + A_{vp1/3} \left( \frac{N^-}{10^{18}} \right)^{1/3} + A_{vp1/2} \left( \frac{N^-}{10^{18}} \right)^{1/2} \quad (784)$$

The total bandgap narrowing is:

$$\Delta E_{gd} = E_{gdc} - E_{gdv} \quad (785)$$

Since the distance between bands shrinks, Eq. 785 gives negative values.

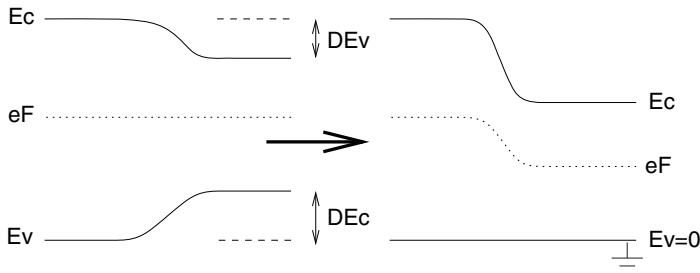


Figure 60 Bandgap narrowing; Sentaurus Process KMC assumes the valence band has zero energy

## Parameters

The parameters  $A_{cn1/4}$  and so on are extracted from [49] and are listed in the parameter database for BandGap in silicon. For the conduction band:

```

pdbGet Si KMC BandGap Acn1.4
0
sprocess> pdbGet Si KMC BandGap Acn1.3
-0.01484
sprocess> pdbGet Si KMC BandGap Acn1.2
0.00078
sprocess> pdbGet Si KMC BandGap Acp1.4
-0.01627
sprocess> pdbGet Si KMC BandGap Acp1.3
0
sprocess> pdbGet Si KMC BandGap Acp1.2
-0.00018

```

For the valence band:

```

sprocess> pdbGet Si KMC BandGap Avn1.4
0.01508
sprocess> pdbGet Si KMC BandGap Avn1.3
0
sprocess> pdbGet Si KMC BandGap Avn1.2
0.00074
sprocess> pdbGet Si KMC BandGap Avp1.4
0
sprocess> pdbGet Si KMC BandGap Avp1.3
0.01846
sprocess> pdbGet Si KMC BandGap Avp1.2
-0.00263

```

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Fermi-Level Effects: Charge Model

## Narrowing due to Strain

The models available for modeling the narrowing due to stress are a simple narrowing model and a full narrowing model.

The full narrowing model is chosen by setting the PDB parameter `Full.Narrowing` to `true`. This model is the same as in [Bandgap Narrowing on page 265](#):

$$\Delta E_{ci} = D_{ci}(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) + D_{cxi}\epsilon_{xx} + D_{cyi}\epsilon_{yy} + D_{czi}\epsilon_{zz} \quad (786)$$

$$\begin{aligned} \Delta E_{vi} = & D_{vi}(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) \pm 0.5D_{vbi}((\epsilon_{xx} - \epsilon_{yy})^2 + (\epsilon_{yy} - \epsilon_{zz})^2 + (\epsilon_{zz} - \epsilon_{xx})^2) \\ & + D_{vdi}(\epsilon_{xy}^2 + \epsilon_{xz}^2 + \epsilon_{yz}^2) \end{aligned} \quad (787)$$

Sentaurus Process KMC also uses the averaged values of the energies of the conduction and valence bands:

$$\Delta E_{cs} = -kT \log \left( \frac{1}{3} \sum_{i=1}^3 e^{-\frac{\Delta E_{ci}}{kT}} \right) \quad (788)$$

$$\Delta E_{vs} = kT \log \left( \frac{1}{2} \sum_{i=1}^2 e^{-\frac{\Delta E_{vi}}{kT}} \right) \quad (789)$$

defining the narrowing due to strain effects as:

$$\Delta E_{gs} = \Delta E_{cs} - \Delta E_{vs} \quad (790)$$

The simple model computes the narrowing as:

$$\Delta E_{gs} = K |\epsilon_x + \epsilon_y + \epsilon_z| \quad (791)$$

where the parameter  $K$  is called `DiScalar`.

When Ge is present, the narrowing is computed as a linear interpolation between the narrowing produced by strain for pure Si ( $\Delta E_{gs}^{\text{Si}}$ ), and the one for pure Ge ( $\Delta E_{gs}^{\text{Ge}}$ ). In this way, the total narrowing for  $\text{Si}_{1-x}\text{Ge}_x$  is:

$$\Delta E_{gs} = \Delta E_{gs}^{\text{Si}} + x(\Delta E_{gs}^{\text{Ge}} - \Delta E_{gs}^{\text{Si}}) \quad (792)$$

where  $x$  is the relative Ge concentration specified in  $\text{Si}_{1-x}\text{Ge}_x$ .

## Parameters

The parameters used for the full model for pure Si are defined in the Sentaurus Process KMC dataset as:

```
sprocess> pdbGet Si KMC BandGap EcDilatational
          1 -8.6
          2 -8.6
          3 -8.6
sprocess> pdbGet Si KMC BandGap EvDilatational
          1 -2.1
          2 -2.1
sprocess> pdbGet Si KMC BandGap EcDeviatoric(1)
          1 9.5
          2 0.0
          3 0.0
sprocess> pdbGet Si KMC BandGap EcDeviatoric(2)
          1 0.0
          2 9.5
          3 0.0
sprocess> pdbGet Si KMC BandGap EcDeviatoric(3)
          1 0.0
          2 0.0
          3 9.5
sprocess> pdbGet Si KMC BandGap EvDeviatoric(1)
          1 0.5
          2 4.0
sprocess> pdbGet Si KMC BandGap EvDeviatoric(2)
          1 0.5
          2 4.0
```

The parameter for the simple model for pure Si is:

```
sprocess> pdbGet Si KMC BandGap DiScalar
          1.75
```

The parameters used for pure Ge are similar to those for pure Si, but with the Ge. prefix:

```
sprocess> pdbGet Si KMC BandGap Ge.EcDilatational
          1 0.59  2 0.59  3 0.59
sprocess> pdbGet Si KMC BandGap Ge.EvDilatational
          1 -1.24 2 -1.24
sprocess> pdbGet Si KMC BandGap Ge.EcDeviatoric(1)
          1 -9.42 2 0.0  3 0.0
sprocess> pdbGet Si KMC BandGap Ge.EcDeviatoric(2)
          1 0.0   2 -9.42 3 0.0
sprocess> pdbGet Si KMC BandGap Ge.EcDeviatoric(3)
          1 0.0   2 0.0   3 -9.42
```

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Fermi-Level Effects: Charge Model

```
sprocess> pdbGet Si KMC BandGap Ge.EvDeviatoric(1)
1 2.55 2 5.50
sprocess> pdbGet Si KMC BandGap Ge.EvDeviatoric(2)
1 2.55 2 5.50
sprocess> pdbGet Si KMC BandGap Ge.DiScalar
1.75
```

Finally, the simple (0) or full (1) narrowing models are selected:

```
sprocess> pdbGet Si KMC BandGap Full.Narrowing
0
```

## Narrowing due to Presence of an Alloy

There are two models to compute bandgap narrowing due to the presence of an alloy: `Simple` and `Braunstein`. The default is set to the `Simple` model.

In the `Simple` model, the narrowing due to an alloy concentration is computed as (assuming, in this example, that Ge is the alloy in Si material):

$$\Delta E_{gGe} = -[Ge](\beta_1 + \beta_2[Ge]) \quad (793)$$

where  $[Ge]$  is the germanium concentration, and  $\beta_1, \beta_2$  are the parameters needed for the quadratic interpolation between the silicon gap (1.12 eV) and the Ge gap (0.78 eV). They are called `GeNarrowing` and `GeNarrowing2`, respectively.

In the `Braunstein` model, the narrowing due to a mole fraction  $x$  of the alloy is computed using the following formula:

$$\Delta E_{gGe} = (0.3758(0.7795 - x)^2 - 0.22835) - 0.2406 \exp\left(-\left(\frac{1-x}{0.1176}\right)^2\right) \quad (794)$$

which has been fitted to the nonlinearity observed in experiments. This model does not use the `GeNarrowing` and `GeNarrowing2` parameters.

## Parameters

```
sprocess> pdbGet Si KMC BandGap Alloy.Narrowing.Model
Simple
sprocess> pdbGet Si KMC BandGap GeNarrowing
6.8e-24
sprocess> pdbGet Si KMC BandGap GeNarrowing2
0
```

This is simply  $(1.12-0.78)/5e22$  for the `Simple` model.

## Bandgap Narrowing Use

The value of  $\Delta E_g$ , computed as:

$$\Delta E_g = \Delta E_{gdop} + \Delta E_{gs} + \Delta E_{gGe} \quad (795)$$

is used to correct  $e_i$ ,  $n_i$ ,  $e_F$ , and the dopant levels in the gap,  $e(j, j+1)(A)$ . For these last ones, they are assumed to be proportional to the band gap. This means that these new values, after applying the bandgap narrowing correction, are:

$$e(j, j+1)(A)^{corrected} = e(j, j+1)(A) \left( 1 + \frac{\Delta E_g}{E_g} \right) \quad (796)$$

It is interesting to note that  $\Delta E_g < 0$ .

Whenever a Sentaurus Process KMC model needs a bandgap level, the bandgap narrowing-corrected value is used. The only exception is the activation energy for the impurity pair emission from impurity clusters where the narrowing correction can be controlled by:

```
pdbSet <material> KMC BandGap Correct.Complex <false | true>
```

**NOTE** The bandgap narrowing due to doping, stress, and SiGe is always switched on by default. To disable it, set the proper parameters to zero.

## Example: Charge Model and Boron Diffusion

The known charge states of  $B_i$  are  $B_i^-$ ,  $B_i^0$ , and  $B_i^+$  [21][22]. The three states are included in Sentaurus Process KMC, although the inclusion of  $B_i^+$  is only important for systems far from equilibrium. The pairing, breakup, and charge reactions related to  $B_i$  are represented in the current Sentaurus Process KMC model by the reactions:



## 5: Atomistic Kinetic Monte Carlo Diffusion

### Fermi-Level Effects: Charge Model

Direct breakup of  $B_i^+$  is not included because  $I^{++}$  is not implemented. Boron effective diffusivity  $D(B)$  is given by the sum of the contribution of all mobile species:

$$D(B) = D(B_i^-) \frac{[B_i^-]}{[B^-]} + D(B_i^0) \frac{[B_i^0]}{[B^-]} + D(B_i^+) \frac{[B_i^+]}{[B^-]} \quad (801)$$

Using the Maxwell–Boltzmann approximation, the previous equation is usually written as:

$$D(B) = S_I \left[ D_X(B) + D_P(B) \frac{p}{n_i} + D_{PP}(B) \left( \frac{p}{n_i} \right)^2 \right] \quad (802)$$

where  $S_I$  is the interstitial supersaturation, and  $p$  and  $n_i$  are the hole concentration and the intrinsic concentration, respectively.

The relations between the above diffusivity components and the microscopic parameters are [48]:

$$D_X(B) = v_{capt} D(I^0) [I^0] * \frac{v_m(B_i^-)}{v_{break}(B_i^-)} \quad (803)$$

$$D_P(B) = v_{capt} D(I^0) [I^0] * \frac{v_m(B_i^0)}{v_{break}(B_i^0)} \exp\left(\frac{e(B_i)(0, -) - e_i}{k_B T}\right) \quad (804)$$

$$D_{PP}(B) = v_{capt} D(I^0) [I^0] * \frac{v_m(B_i^+)}{v_{break}(B_i^+)} \exp\left(\frac{e(B_i)(0, -) + e(B_i)(+, 0) - 2e_i}{k_B T}\right) \quad (805)$$

$e_i$  is the intrinsic level.

These expressions can be used as a bridge between the parameters of continuum simulators and those used by Sentaurus Process KMC. The above continuum expression assumes Maxwell–Boltzmann and quasi-equilibrium conditions, which are not needed in Sentaurus Process KMC.

## Example: Charge Model and Arsenic Diffusion

A similar analysis can be performed for arsenic, which has both vacancy and interstitial contributions, related to AsV and  $As_i^+$  defects. The arsenic reactions are:





and:



All the previously mentioned contributions are included in Sentaurus Process KMC. Consequently:

$$D(As) = D(AsV^+) \frac{[AsV^+]}{[As^+]} + D(As_i^+) \frac{[As_i^+]}{[As^+]} + D(AsV^0) \frac{[AsV^0]}{[As^+]} + D(As_i^0) \frac{[As_i^0]}{[As^+]} + D(AsV^-) \frac{[AsV^-]}{[As^+]} \quad (815)$$

which in continuum models is usually reduced to:

$$D(As) = [f_I S_I - (1-f_I) S_V] \times \left[ D_X(As) + D_M(As) \frac{n}{n_i} + D_{MM}(As) \left( \frac{n}{n_i} \right)^2 \right] \quad (816)$$

$f_I$  is the fraction of interstitial-assisted diffusion. Note, however, that this last continuum description conveys several simplifying assumptions compared with the model included in Sentaurus Process KMC. The common assumption that  $D_X$  and  $D_M$  fit an Arrhenius plot is only true if the contributions of  $AsV^+$  and  $As_i^+$  have the same activation energy. The same applies to the  $AsV^0$  and  $As_i^0$  contributions. The continuum equation also assumes that the interstitial fraction,  $f_I$ , is independent of the Fermi level (the same for the three charge states) and is independent of the temperature.

## Interfaces and Surfaces

An interface is the extension between two regions with different materials. The silicon–oxide interface is the most common interface. Sentaurus Process KMC can model all interfaces between two different materials.

As explained in [Materials and Space on page 391](#), Sentaurus Process KMC divides the space in small rectangular elements and assigns a material to each of them. The interfaces are the set of element faces between different materials.

The element faces are independent. The interface behaves as the sum of all of its faces, but such an ‘interface’ does not really exist. What exists are the element faces, all of them emitting and trapping with different rates depending on its area, local stress, and so on. In the following sections, these element faces are called *interfaces*.

Interfaces set the equilibrium concentration for self-silicon point defects and the solubility concentration for impurities. Sentaurus Process KMC models the interfaces differently for silicon point defects than for impurities.

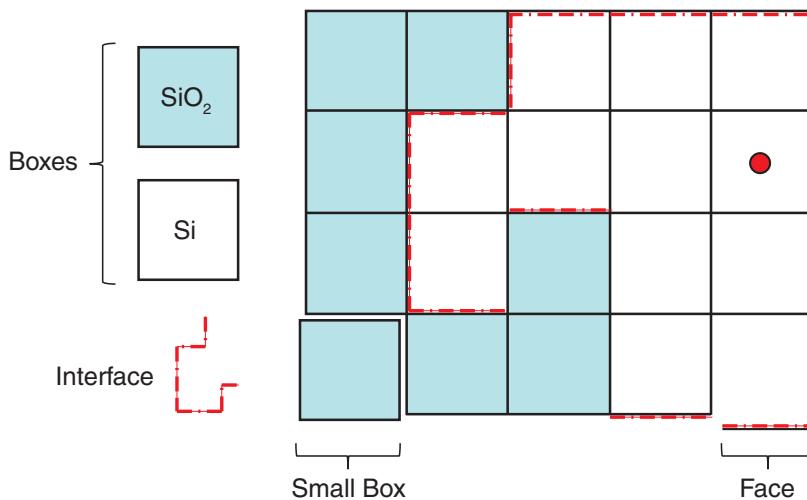


Figure 61 Sentaurus Process KMC interfaces are the set of element faces between different materials

---

## Interface Models

The parameter `Model` specifies the behavior of an interface:

```
pdbSet Oxide_Silicon KMC Model <model>
```

where `<model>` can be one of the following:

Allcharges	Three-phase segregation model for dopants. Emission and capture of all the charge states of point defects on materials with <code>full</code> modeling. Capture of all the charge states of impurity-paired defects on materials with <code>full</code> modeling.
Amorphous	When one material is <code>full</code> and the other is <code>simple</code> , this interface acts as an asymmetric mirror. Particles going from the <code>simple</code> to the <code>full</code> material are reflected, while particles going from the <code>full</code> to the <code>simple</code> material are allowed to pass. No trapping or emission of particles on either side.
Interface	Three-phase segregation model for dopants. Emission and capture of neutral point defects on materials with <code>full</code> modeling.
None	No interface between materials. This model is possible only when the model of the materials involved in the interface is the same, that is, both are <code>simple</code> or <code>full</code> .
Reflective	The interface acts as a mirror. Particles are not trapped, and there is no emission of particles on either side.

---

## Interfaces for Self-Silicon Point Defects

It is common to define a recombination length  $L_r$  as the distance from the surface needed to obtain the equilibrium concentration (see [Figure 62 on page 508](#)).

The microscopic meaning of  $L_r$  can be associated with the probability of a point defect being trapped at the surface:

$$P_{trap} = \frac{\lambda}{L_r} \quad (817)$$

where  $\lambda$  is the point-defect jumping distance. The smaller  $L_r$ , the better sink is the surface. For interstitials in the silicon–oxide interface, it is close to a perfect sink with  $L_r < 5$  nm [\[51\]\[52\]](#).

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Interfaces and Surfaces

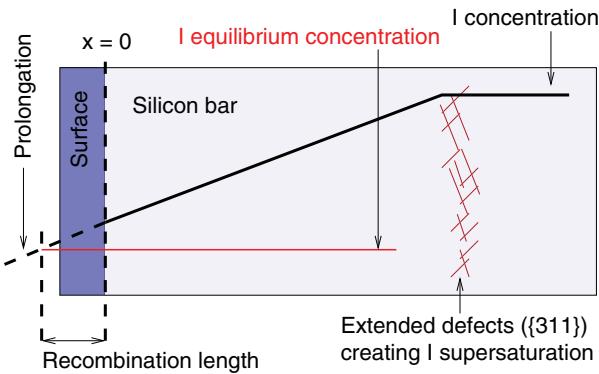


Figure 62 Recombination length is the distance between the interface and the point in which the prolongation of the point-defect concentration joins its equilibrium concentration

## Capture

Interfaces capture neutral interstitials and vacancies with the probability set in Eq. 817. When  $L_r$  is set to zero, the probability is set to 1, that is, a perfect sink.

## Emission

In [1], the point-defect (for example, interstitials) equilibrium concentration is related to the interface frequency emission prefactor and energy as:

$$[I]^* = \frac{2}{\lambda} \times \frac{D_0 FS}{a^2} \exp\left(-\frac{E_f(I)}{k_B T}\right) \quad (818)$$

where the surface frequency emission is:

$$v = \text{sites} \times P_{trap} \times D_0 FS \frac{6}{\lambda^2} D_{0,m} \times \exp\left(-\frac{E_m + \Delta E_m^{stress} + \Delta E_m^{Ge} + E_f + \Delta E_f^{stress} + \Delta E_f^{Ge}}{k_B T}\right) \quad (819)$$

where:

- $\text{sites}$  is the number of capture sites in the interface (proportional to its surface and equal to  $\frac{2}{a^2} YZ$ ).
- $D_0 FS$  is the surface emission prefactor.
- $E_m$  and  $E_f$  are the migration and formation energies of the point defects, respectively.

- $\Delta E_m^{\text{stress}}$ ,  $\Delta E_f^{\text{stress}}$  are the regular corrections to migration and formation due to stress.
- $\Delta E_m^{\text{Ge}}$ ,  $\Delta E_f^{\text{Ge}}$  are the corrections to migration and formation due to Ge concentration, explained below.

The point defects are emitted from a randomly chosen position at the surface. Only neutral *I*s or *V*s are emitted when the interface model is `Interface`. All charge states are emitted and captured when using the `Allcharges` model. In equilibrium, these two models give the same results.

## Stress

The presence of stress changes the migration and formation energies of interstitial and vacancies and, consequently, the emission frequency. Each interface (where, as previously stated, interface was called to the independent element faces) is oriented in a unique axis *j*, and the projections of the principal axes into *j* should be accounted for. Then, the total emission frequency is:

$$v = \sum_{\text{axis}} P_{\text{axis}}^j v_{\text{axis}} \quad (820)$$

where  $P_{\text{axis}}^j$  are the projections of the principal axis into the surface axis. Finally, for each axis, the migration and formation energies including stress effects are computed as:

$$E_m^{\text{stress}} + E_f^{\text{stress}} = E_m + E_f + \sigma'_{\text{axis}} \Delta V_{\text{par}} + \sum_{i \neq \text{axis}} \sigma'_i \Delta V_{\text{ort}} + \frac{1}{3} \Delta V^f \sum_i \sigma'_i \quad (821)$$

where  $\Delta V_{\text{ort}}$  and  $\Delta V_{\text{par}}$  are the perpendicular and parallel activation volumes for diffusion, respectively, and  $\Delta V^f$  is the activation volume for formation.

For more information on these parameters and the stress models, see [Stress Effects on Point Defects, Impurities, Dopants, and Impurity-Paired Point Defects on page 422](#).

## Alloys

The presence of an alloy (assumed to be Ge in this example) changes the migration and the formation energy of point defects in the following way, when parameter interpolation is not switched on:

$$\begin{aligned} \Delta E_m^{\text{Ge}} &= \alpha[\text{Ge}] \\ \Delta E_f^{\text{Ge}} &= \beta[\text{Ge}] \end{aligned} \quad (822)$$

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Interfaces and Surfaces

where  $[Ge]$  is the germanium concentration, and  $\alpha, \beta$  are the dependencies of migration and formation with germanium, specified as `EmGe` and `EfGe` in the PDB. When parameter interpolation is switched on, these parameters are interpolated directly between the component materials of the alloy.

## Parameters

The parameters that control the point-defect interface model can be found in the PDB by looking in the `Oxide_Silicon` folder. By default, interfaces, other than the oxide–silicon interface, have their point-defect interface model set to `None` and do not require any parameters. The formation energies are listed for the material, not for the interface.

For example, the formation energy of interstitials in silicon is under `Silicon`, not in `Oxide_Silicon` or any other interface.

`D0FS_Mat`      Surface emission prefactor,  $D_0FS(I)$ . `Mat` is the full name of the material.  
`Ef`               Formation energy,  $E_f(I)$ .  
`RecLnm_Mat`    Recombination length,  $L_r$ . `Mat` is the full name of the material.

The migration energies are displayed in the point-defect section of the file (see [Point Defects, Impurities, Dopants, and Impurity-Paired Point Defects on page 408](#)). The surface values can be easily obtained using the command line.

For example, for interstitials and vacancies in the silicon–oxide interface:

```
sprocess> pdbGet Oxide_Silicon KMC I D0FS_Silicon  
5000.0  
sprocess> pdbGet Silicon KMC I Ef  
4.0  
sprocess> pdbGet Oxide_Silicon KMC I RecLnm_Silicon  
0  
sprocess> pdbGet Oxide_Silicon KMC V D0FS_Silicon  
800.0  
sprocess> pdbGet Silicon KMC V Ef  
3.8  
sprocess> pdbGet Oxide_Silicon KMC V RecLnm_Silicon  
0
```

and for vacancies in the silicon–gas interface:

```
sprocess> pdbGet Gas_Silicon KMC V D0FS_Silicon  
800.0  
sprocess> pdbGet Gas_Silicon KMC V RecLnm_Silicon  
0
```

```
sprocess> pdbGet Si KMC V Ef
3.8
```

**NOTE** You can modify these values. Changes in the formation energy or surface emission prefactor will modify the diffusion coefficient (DC) equilibrium product of point defects and the diffusivity of all the species. A change, both in the formation and migration parameters, that maintains the DC product constant will not produce this undesirable effect, but may change the extended defects dissolution times.

## Oxidation-Enhanced Diffusion (OED) Model

The current flux of I (V) across an outer surface in Sentaurus Process KMC is described in the previous model as:

$$\vec{j} \cdot \vec{n} = K_s([I] - [I^*]) \quad (823)$$

being:

$$K_s = \frac{1}{6} v_m(I) \lambda^2 / L_r \quad (824)$$

and  $\lambda$  the jumping distance. An extra term is included to account for oxidation:

$$\vec{j} \cdot \vec{n} = K_s([I] - [I^*]) - G_{ox} \quad (825)$$

The term  $G_{ox}$  tries to combine the Sentaurus Process continuum model (see [Surface Recombination Model: PDependent on page 345](#)) with an atomistic implementation. In particular, its definition is:

$$G_{ox} = (\vec{\theta} \cdot \vec{n}) \left\| \vec{V}_{ox} \right\| G_{scale} \left( \frac{\left\| \vec{V}_{ox} \right\|}{V_{scale}} \right)^{G_{pow}} \exp \left( -\frac{E_\theta + P \Delta V_\theta}{k_B T} \right) \quad (826)$$

where:

- $\vec{\theta}$  is a vectorial prefactor and  $\vec{n}$  is the normal to the interface, so that  $(\vec{\theta} \cdot \vec{n})$  gives the proper component for a planar, axis-oriented, interface in an internal element.
- $\left\| \vec{V}_{ox} \right\|$  is the ReactionSpeed computed by the PDE solver in Sentaurus Process and used here by Sentaurus Process KMC.
- $V_{scale}$  and  $G_{pow}$  are additional model parameters to adjust the interstitial injection.

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Interfaces and Surfaces

- $G_{scale}$  is a term defined to account for Fermi-level effects, and defined similarly to the continuum one as:

$$G_{scale} = \frac{mm + m + 1 + p + pp}{mm\left(\frac{n}{n_t}\right)^{2PotOx} + m\left(\frac{n}{n_t}\right)^{PotOx} + 1 + p\left(\frac{n}{n_t}\right)^{-PotOx} + pp\left(\frac{n}{n_t}\right)^{-2PotOx}} \quad (827)$$

- $E_\theta$  is the activation energy for point-defect injection.
- $\Delta V_\theta$  is a parameter to include a hydrostatic dependency for OED.

Consequently, this is a hybrid model in which the continuum solver computes and generates a ReactionSpeed value to be used by Sentaurus Process KMC to compute the point-defect injection prefactor.

**NOTE** Boundary movement is allowed in this model and is switched on by default. This implies that the model serves to generate a more adequate point-defect injection from the interface during oxidation processes, while a remeshing mechanism changes the oxide thickness. If you do not want the oxide thickness to change, set:

```
pdbSet Grid Reaction.Modify.Mesh 0
```

**NOTE** Point-defect injection during nitridation in Sentaurus Process KMC also can be simulated similarly to the OED model, using the same set of parameters (see [Table 62](#)). For defect injection to occur during nitridation, you must set the parameter Oxide to true in Nitride material, for example:

```
pdbSet Nitride KMC Oxide true
```

[Table 62](#) lists the parameters defined for the oxide–silicon interface and for the nitride–silicon interface.

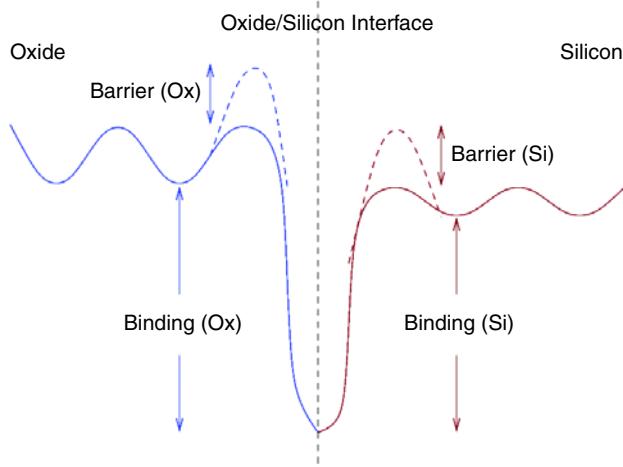
Table 62 Parameters used in OED model (and defect injection during nitridation)

Parameter	Description
Injection.Etheta	Activation energy $E_\theta$ .
Injection.Xtheta, Injection.Ytheta, Injection.Ztheta	Components for the $\vec{\theta}$ vector used as a prefactor.
Injection.VFtheta	Pressure correction $\Delta V_\theta$ .
Injection.Vscale, Injection.Gpow	ReactionSpeed control: $V_{scale}$ and $G_{pow}$ .
Injection.PP, Injection.P, Injection.EP, Injection.M, Injection.MM, Injection.EM, Injection.Pot	Parameters used to compute the Fermi-level dependencies introduced by $G_{scale}$ . In particular, prefactor and activation energies for $pp$ , $p$ , $m$ , and $mm$ terms, and exponent.

To use this model, use the `diffuse` command with any oxidation parameter (for a list of oxidation parameters for `diffuse`, see [diffuse on page 935](#)).

## Interfaces for Impurities

The interface model of impurities in Sentaurus Process KMC follows the three-phase segregation model. Particles can be emitted to both sides of the interface or can stay trapped at the interface. [Figure 63](#) shows the atomistic mechanisms and energies for trapping and detrapping impurities.



**Figure 63** Dopants reaching the interface may be trapped there with a different binding energy for each interface side; energy barriers for capture and emission also can be present

These interfaces are modeled between any two materials. However, depending on the material model, the interface will behave differently.

### Simple Material Side

The simple material side faces a material that uses the `simple` model. In these materials, only direct diffusion of dopants is allowed. Since there are no paired dopant impurity point-defects, the model is as follows: Dopants arriving at the nonsilicon side may be captured with certain probability, and they can be remitted later.

#### Capture

The capture probability is:

$$P_{cap(A)}^{non-Si} = \exp(-\text{Barrier}(A)/(k_B T)) \left( 1 - \frac{\text{Trapped}(A)}{\text{MaxTrapped}(A)} \right) \quad (828)$$

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Interfaces and Surfaces

where  $A$  is the dopant being trapped,  $Barrier$  is the barrier energy,  $Trapped$  is the number of particles trapped at the interface, and  $MaxTrapped$  is the maximum number of them that can be trapped.

If the particle is trapped, there is a probability to evaporate (annihilate) the just-trapped dopant.

### Emission

Interfaces emit particles to the nonsilicon side with a frequency given by:

$$v_{emiss}^{\text{non-Si}}(A) = Trapped(A)Pref \exp(-Ener/(k_B T)) \quad (829)$$

The emission is proportional to the number of trapped dopants and to a parameter `Pref` that acts as a prefactor. The emission energy is:

$$Ener(A) = Barrier(A) + E_m(A) + Binding(A) \quad (830)$$

The migration energy contains stress and Ge corrections. The binding energy contains a pressure correction:

$$\Delta E_b^{surface}(A) = P \Delta V_b^{surface}(A) \quad (831)$$

### Parameters

The energy barrier to a nonsilicon interface is introduced as `EBARRIER_<mat>`, where `<mat>` is the name of one of the sides of the interface.

The values are always specified in the interface parameter file:

```
sprocess> pdbGet Oxide_Silicon KMC B EBarrier_Oxide  
B 0.1
```

The probability to evaporate a trapped particle is called `Evaporation.Surf`:

```
sprocess> pdbGet Oxide_Silicon KMC B Evaporation.Surf  
B 0 Bi 0
```

The pressure correction to the binding energy of the dopants to the surface is given by the parameter `VF_<mat>`:

```
sprocess> pdbGet Oxide_Silicon KMC B VF_Oxide
```

The maximum number of trapped particles per cubic centimeter follows an Arrhenius plot with prefactor `C0Max.Surf`:

```
sprocess> pdbGet Oxide_Silicon KMC B C0Max.Surf  
2e+14
```

and energy EMax.Surf:

```
sprocess> pdbGet Oxide_Silicon KMC B EMax.Surf
0
```

The factor to control dopant (boron) segregation in the presence of another impurity (fluorine) at the interface is called Factor.Max.Surf:

```
sprocess> pdbGet Oxide_Silicon KMC B Factor.Max.Surf
F 1e-12
```

The exponential term for the same is Exp.Max.Surf:

```
sprocess> pdbGet Oxide_Silicon KMC B Exp.Max.Surf
F 1.0
```

The prefactor for emission is called Db.Surf:

```
sprocess> pdbGet Oxide_Silicon KMC B Db.Surf
B 1e-3
```

Finally, the binding energy of dopants is Eb\_<mat>:

```
sprocess> pdbGet Oxide_Silicon KMC B Eb_Oxide
B 0.28
```

## Full Material Side

The particles transporting dopants (or impurities) in materials with full modeling are not typically the dopants themselves, but impurity-paired point defects. In other words, an impurity plus an interstitial or a vacancy. When these *pairs* reach the interface, if they are trapped, the accompanying interstitial or vacancy is recombined, and the dopant itself is piled at the surface. Consequently, the dopant cannot be emitted unless an incoming interstitial or vacancy reacts with it, carrying it away from the interface.

### Capture

Neutral (or charged, if the model Allcharges is selected) impurity-paired point defects are trapped at the surface with a probability given by:

$$P_{cap}^{Si}(A_i) = \exp(-\text{Barrier}(A_i)/(k_B T)) \left( 1 - \frac{\text{Trapped}(A)}{\text{MaxTrapped}(A)} \right) \quad (832)$$

Different barriers can be assigned to  $A_i$  and  $AV$  and, consequently, different recombination probabilities. The number of trapped particles and the maximum number of trapped particles are assigned to the interface and are shared between both sides.

Sentaurus Process KMC also allows shared trapping at interfaces. It essentially means that the presence of a certain impurity may enhance or reduce the trapping of another impurity. This can be controlled using the parameters `Factor.Max.Surf` and `Exp.Max.Surf`. Self-dependency in this case is not allowed. The allowed maximum trapped concentration for impurity  $B$  at the interface in the presence of impurity  $A$  would then be:

$$\text{MaxTrapped}(B, A) = (1 + \text{factor}(B, A) \times \text{Trapped}(A)^{\text{exponent}(A, B)}) \times \text{MaxTrapped}(B) \quad (833)$$

## Emission

Particles are not emitted by themselves, but the interface allows particles to move to the material bulk. Point defects (interstitials and vacancies) can react with dopants trapped at the surface, forming mobile impurity-paired point defects. The probability of these reactions being successful depends on the binding of the dopant to the surface and the barrier energy:

$$P_{\text{emiss}}^{\text{Si}}(A_i) = \exp(-E_{\text{ener}}(A_i)/(k_B T)) \quad (834)$$

where  $E_{\text{ener}}(A_i) = \text{Binding}(A_i) + \text{Barrier}(A_i)$ .

The binding is corrected with a pressure-dependent term:

$$\Delta E_b^{\text{surface}}(A_i) = P \Delta V_b^{\text{surface}}(A_i) \quad (835)$$

## Parameters

The parameters that control the maximum number of trapped particles are discussed in [Simple Material Side on page 513](#). The barrier energy is called `EBarrier_Silicon`:

```
sprocess> pdbGet Oxide_Silicon KMC As EBarrier_Silicon
Asi 0.0
AsV 0.0
```

and the binding energy is `Eb_Silicon`:

```
sprocess> pdbGet Oxide_Silicon KMC As Eb_Silicon
Asi 0.1
AsV 0.1
```

The stress correction is given by:

```
sprocess> pdbGet Oxide_Silicon KMC B VF_Silicon
```

**NOTE** Negative parameter values for `EBarrier_<mat>` and `Eb_<mat>` are allowed at interfaces, which can help to enhance impurity segregation at interfaces.

## Oxidation

Sentaurus Process KMC is fully coupled with oxidation. Consequently, any oxidation conditions issued in the `diffuse` command of Sentaurus Process are transferred to Sentaurus Process KMC.

Setting `Grid Reaction.Modify.Mesh 0` (it is 1 by default) disables boundary movement at the oxide–silicon interface. Otherwise, the Sentaurus Process oxidation algorithm can work during the *reaction* step, and the new structure (with expanded oxide) is imported into Sentaurus Process KMC immediately before the atomistic diffusion step. The velocities at which the interfaces and the oxide move are used to compute the displacement of the particles.

Sentaurus Process KMC uses the displacement to relocate the displaced particles and finishes the remeshing. After this, regular atomistic diffusion occurs. Since there are several interpolations performed in this process, minor inaccuracies in the final position of particles can be introduced during remeshing, especially during large oxidations. Regular diffusion occurring at the same time as oxidation should make these interpolation inaccuracies negligible.

In principle, Sentaurus Process KMC can be used successfully for 1D, 2D, and 3D oxidation. Since the precision of the Sentaurus Process KMC solution does not depend on a fine continuum mesh, a coarse Sentaurus Process mesh can be specified, increasing the stability of oxidation, while the Sentaurus Process KMC part takes care of the position of particles. [Figure 64](#) shows the results of such an approach.

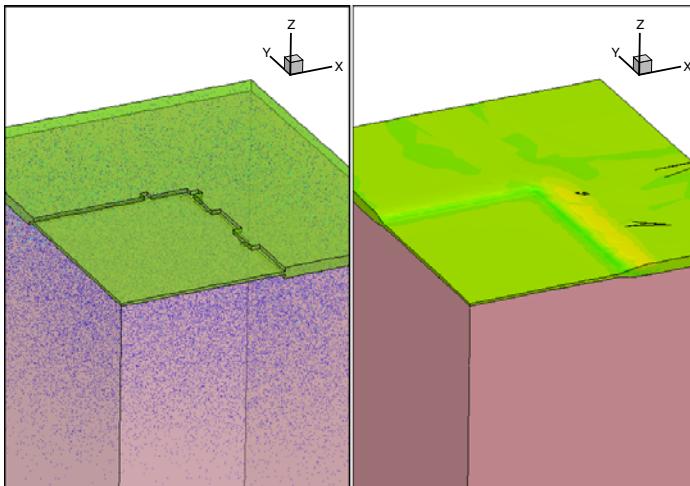


Figure 64 Example of Sentaurus Process KMC coupled with an oxidation in three dimensions: (*left*) KMC simulation in which the internal mesh is coupled to (*right*) continuum oxidation simulation

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Silicidation

Sentaurus Process KMC also allows OED (see [Oxidation-Enhanced Diffusion \(OED\) Model on page 511](#)).

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## Silicidation

Sentaurus Process KMC allows silicide growth by linking with the continuum silicidation model. Nickel silicide and titanium silicide are defined by default in the KMC materials list. Other silicide materials can be added by defining them as new materials and setting them to true for Sentaurus Process KMC.

The `Pref.GrowthDeposit` and `Ener.GrowthDeposit` parameters allow you to control the redistribution of doping from the growing silicide to the substrate silicon.

The probability of dopant transfer to silicide is calculated using the following Arrhenius expression:

$$p = \text{Pref.GrowthDeposit} \times \exp\left(-\frac{\text{Ener.GrowthDeposit}}{kT}\right) \quad (836)$$

Allowed values of `Pref.GrowthDeposit` are between 0 and 1. By default, this value is 1. The default value of `Ener.GrowthDeposit` is 0, thereby giving a default effective probability for dopant transfer into silicide equal to 1. These parameters can be obtained as follows:

```
sprocess> pdbGet NickelSilicide_Silicon KMC Boron Pref.GrowthDeposit  
1.0  
  
sprocess> pdbGet NickelSilicide_Silicon KMC Boron Ener.GrowthDeposit  
0.0
```

---

## Including New Impurities

You can customize Sentaurus Process KMC to include impurities that are not supported by default. The modifications affect the parameter database and the `KMC.tcl` file. Nevertheless, it is not necessary or recommended to modify the files included in the Sentaurus Process distribution. All the modifications can be included in the command file.

For the parameter database, the `pdbSet` family of commands allows overwriting previous values or defining new ones. For the procedures written in the `KMC.tcl` file, defining a new procedure in the command file is sufficient; the new one will be executed instead of the old one.

The modifications include the following:

1. Include the new impurity x in Sentaurus Process KMC under the `KMC Impurities` label.
2. Include the impurity-related particle pairs (`xi` or `xv` or both) in `KMC Pairs` (see [Particles in Models on page 403](#)). If your model does not have impurity pairs (in other words, simple material), you do not need to specify them, including `Dm` and `Em`.
3. Be careful about which charge states you include because not all are allowed. You must specify parameters for all those included.
4. Include possible aliases for the particle in `KMC Aliases`. If the particle already exists for Sentaurus Process, include this name as an alias in Sentaurus Process KMC (see [Aliases of Particle Names on page 404](#)).
5. (Optional) Customize the colors for this particle in Sentaurus Visual in `KMC Colors` (see [Colors of Particles on page 404](#)).
6. Define parameters for the new particle, as explained in [Particles and Parameters on page 404](#), under `KMC <mat> X`, where `<mat>` is every material defined in your simulation, and x is the name of the new defined dopant. Be sure to include all of them. Parameters for the impurity cluster model are not needed if `Implement.Complex` is set to `false`. All others require values since they specify how the surface and amorphous regions interact with the new dopant x.
7. Specify the reactions for `KMC <mat> X` in `ReactionsPointDefect`. Typical reactions here include pair formation (such as `X, I true`) and impurity cluster formation (such as `Xi, X true`). These reactions only need to be defined in materials with the `full` model.
8. Specify also the reactions with damage and extended defects if there are any. You can leave these fields empty. See [Interaction With Impurities on page 437](#), [Interactions on page 441](#), [Interactions on page 446](#), and [Interactions on page 449](#).

If you include impurity clusters, ensure the following:

1. Define reactions that create impurity clusters from two isolated particles.
2. Enable the right impurity clusters for your simulation with `Implement.Complex` (see [Impurity Clusters on page 470](#)).
3. Define the parameters for the impurity clusters. You can leave the energy barriers empty, but you must specify `Etotal.Complex` energies and `CaptVol.Complex` capture volumes.
4. Write the reactions for your impurity clusters. If you have specified an energy for a particular impurity cluster, then that impurity cluster should be reachable through some reactions. Include the reactions with dopants and point defects in `ReactionsCluster` (see [Interactions of Impurity Cluster Model on page 485](#)).
5. If you need dopant deactivation without diffusion for high concentrations, see [Percolation on page 475](#).

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Including New Impurities

Finally, you must define some variables set in the `KMC.tcl` file placed in `TclLib`. This can (and should) be performed locally in your command file:

1. Add the names of your new impurities and pairs to the `nameOf` array.
2. Complete the map of MC implantation to Sentaurus Process KMC with `MCnameOf`.

If you need to transfer information back and forth from continuum to KMC simulations, you also must modify the procedures `PDE2KMCUser` and `KMC2PDEUser`:

- Add the new particles and clusters to the lists in `PDE2KMCUser`. The first field is the field name in Sentaurus Process (continuum models), the second is the name in Sentaurus Process KMC, and the third is the conversion factor. For example:

```
fproc PDE2KMCUser {} {  
    return "Dopant X 1 \  
    DopantInt Xi 1 \  
    DopantVac XV 1 \  
    DopantCluster X2 .5 \  
    DopantCluster X3 .3333"  
}
```

- Add the new particles in `KMC2PDEUser`. The first name is the name in Sentaurus Process KMC, the second is the Sentaurus Process field, and the third is the factor. For example:

```
fproc KMC2PDEUser {} {  
    return "X Dopant 1\  
    Xi DopantInt 1\  
    XV DopantVac 1\  
    X2 DopantCluster 1\  
    X3 DopantCluster 1.5\  
    X4 DopantCluster 2"  
}
```

**NOTE** `MCnameOf` can be used to manipulate some KMC species without actually implementing them. For example, an unknown implantation can be performed to simulate preamorphization. If Sentaurus Process KMC does not support the unknown dopant, use `set MCnameOf(dopant) "I"` to instruct Sentaurus MC to pass the dopant atoms as interstitials to Sentaurus Process KMC. This way, all of the damage generated by an unknown dopant implantation will be correctly calculated and passed, and the dopant ions will be considered to be silicon interstitials by Sentaurus Process KMC.

## Impurities Diffusing Without Pairing

Sentaurus Process KMC allows impurities to diffuse using two different mechanisms:

- Normal diffusion
- Diffusion without pairing

### Normal Diffusion

For impurities with +1 or -1 charge (that is, dopants), the substitutional dopant is active, but it does not diffuse. The substitutional dopant reacts with interstitials or vacancies, forming a pair that diffuses. These pairs break up with a given frequency, releasing the dopants back into the substitutional positions.

### Diffusion Without Pairing

For neutral impurities, normal diffusion is still available. An alternative diffusion mechanism is migration without pairing. In these cases, the impurity diffuses as it is, that is, the substitutional impurity has a nonzero diffusivity and continues forming pairs with point defects.

Diffusion without pairing has the following characteristics:

- The impurity has nonzero diffusivity. Pairs can exist, but they do not have to diffuse:

```
sprocess> pdbGet Silicon KMC F Dm
          F 5e-3
          FV 0
          FI 0
sprocess> pdbGet Silicon KMC F Em
          F .8
          FV 5
          FI 5
```

- When a pair (for example, FI) breaks up, [Eq. 687](#) and [Eq. 688, p. 413](#) still apply. The migration energy of the impurity is not accounted for.
- The impurities cannot interact with extended defects, but their pairs can, as explained in [Extended Defects on page 438](#).
- Impurities interact with interfaces. Interfaces re-emit impurities.
- Impurity clusters are possible with some variations:
  - Reactions within the impurities (for example,  $F + F$ ) apply to the moving particles and not only the percolation model.

- Impurity clusters emit point defects and impurities, as explained in [Emission on page 431](#), but the capture and emission reactions for impurities are:



- Consequently, the binding energies involved in the capture and emission of impurities will be:

$$E^{A_n I_m}_b(A) = E_{pot}(A_{n+1} I_m) - E_{pot}(A_n I_m) \quad (838)$$

- Recombination, FT, and complementary FT mechanisms are implemented as well. The binding energies for them are not changed since the emission recombination of  $A_i$  (for  $A_n I_m$  clusters) or AV (for  $A_n V_m$  clusters) is not involved.

---

## Reports

Sentaurus Process KMC prints different reports in the log file including:

- Models used
- Particle distribution
- Cluster distribution
- Defect activity
- Interactions
- Event

---

## Models Used Report

Sentaurus Process KMC reports the models used immediately after being initialized. This summary is printed for any particle allowed in the simulation, even if the particle will not be used:

KMC models	Silicon
+-----+	+-----+
Interstitial	
DiffModel	Direct(I)
ChargeModel	I( -1 0 1 )
ClusterModel	I+I AmorphousPocket Void ThreeOneOne Loop
SPERModel	Clean
Vacancy	
DiffModel	Direct(V)
ChargeModel	V( -2 -1 0 1 2 )

	ClusterModel	V+V AmorphousPocket Void ThreeOneOne
	SPERModel	Clean
Arsenic		
	DiffModel	Kick-out (Asi) Kick-out (AsV)
	ChargeModel	Asi( 0 1 ) AsV( -1 0 1 )
	ClusterModel	As+As AsnVm
	SPERModel	As4Vm 30% deposited 70% moved
Boron		
	DiffModel	Kick-out (Bi)
	ChargeModel	Bi( -1 0 1 )
	ClusterModel	BnIm AmorphousPocket Loop
	SPERModel	B3Im 100% deposited 0% moved
Fluorine		
	DiffModel	Direct(F)
	ChargeModel	FI( 0 ) FV( 0 )
	ClusterModel	F+F FnIm FnVm
	SPERModel	F2Im F2Vm 30% deposited 70% moved
-----		
	Stress model	Disable
-----		
	SPER model	Non-Lattice KMC
-----		

Table 63 Sentaurus Process KMC models

Model	Description
ChargeModel	The particles and their allowed charge states are displayed.
ClusterModel	The interactions between the impurity or point defect and extended defects and clusters are displayed.
DiffModel	The diffusion model can be direct or kick-out. Kick-out means that the particle does not diffuse unless paired with an interstitial or a vacancy.
SPERModel	Recrystallization model shows the percentage of dopant being deposited, and the bigger deposited cluster, if any. Point defects are solely cleaned during the recrystallization.
Stress model	This is either disabled or enabled.
SPER model	The algorithm for SPER can be nonlattice KMC (isotropic) or lattice KMC (anisotropic).

## Particle Distribution Report

The particle distribution report lists how many dopants exist per material and the state of the material:

```
--          KMC Particle distribution report
Material      Dopant   Total   State
Nitride       As        28604    100.00% mobile
```

## 5: Atomistic Kinetic Monte Carlo Diffusion Reports

Oxide	As	759	100.00%	mobile
Oxide_Silicon	As	1777	100.00%	trapped
PolySilicon	As	21986	100.00%	mobile
Silicon	As	58394	41.55%	active
Oxide	B	25	100.00%	mobile
PolySilicon	B	283	100.00%	mobile
Silicon	B	828	99.52%	active

The different states depend on the material:

- full material      Particles can be active (substitutional dopant) or inactive (anything else).
- simple material    Particles can be mobile (single impurity) or immobile (impurity in a cluster).
- Interface          Number of particles trapped at the interface.

---

## Cluster Distribution Report

This report shows the distribution of clusters versus size for each material and reports how many clusters are in the simulation and their types:

```
--          KMC impurity cluster distribution report  --
Name      #number
--- Silicon ---
As4I      4889 As2        4062 As4        1110 As2V      571
As3I      121  As2I       95  As3        56  As3V      19
As4V      9   As4I2       6   B2I2        2
```

For example, in the above report, all the BICs are  $B_2I_2$ . The As–vacancy clusters are distributed between different types, but the most common one is  $As_4I$ .

---

## Defect Activity Report

Sentaurus Process KMC displays the point defects, impurities, dopants, extended defects, clusters, amorphous areas, recrystallizations, and surface emission accounted for during the simulation:

```
--          KMC defect activity report  --
First:  Time Events Temp | Last: Time     Events Temp Label
      0.000 0.00e+00 27 |           3e-01 2.86e+09  672 PointDefect (I)
      0.000 0.00e+00 27 |           2e-01 2.86e+09  772 PointDefect (V)
2.285897e-02 1.04e+06 27 |           75610 here                  PointDefect (As)
      0.000 0.00e+00 27 |           1132 here                  PointDefect (B)
```

9.639	1.47e+06	27		4e-01	2.86e+09	572	PointDefect	(IM)
1.657462e-01	1.08e+03	27		3e-01	2.86e+09	672	PointDefect	(IP)
11.025	1.52e+06	27		2e-01	2.86e+09	722	PointDefect	(VMM)
2.849592e-02	3.60e+01	27		2e-01	2.86e+09	722	PointDefect	(VM)
103.606	2.99e+06	27		2e-01	2.86e+09	772	PointDefect	(VP)
2.352941e-04	1.19e+07	650		1e-03	1.85e+09	1230	PointDefect	(VPP)
6.114947e-01	1.08e+06	27		2e-01	2.86e+09	722	PointDefect	(AsV)
13.397	1.60e+06	27		2e-01	2.86e+09	722	PointDefect	(AsVM)
6.057627e-01	1.08e+06	27		2e-01	2.86e+09	772	PointDefect	(AsVP)
0.000	1.04e+06	27		8e-01	2.86e+09	222	PointDefect	(Asi)
8.988	1.45e+06	27		33	here		PointDefect	(AsiM)
9.790420e-01	1.10e+06	27		4e-01	2.86e+09	622	PointDefect	(AsiP)
9.143608e-01	2.14e+04	27		6e-04	2.55e+07	1000	PointDefect	(BV)
1.154401e-01	5.63e+02	27		1e-03	1.68e+09	1230	PointDefect	(BVM)
1.501662e-01	9.14e+02	27		7e-04	3.78e+07	1040	PointDefect	(BVP)
0.000	0.00e+00	27		3e-01	2.86e+09	672	PointDefect	(Bi)
7.337895e-03	2.00e+00	27		3e-01	2.86e+09	672	PointDefect	(BiM)
1.501662e-01	9.14e+02	27		1e-03	7.36e+08	1300	PointDefect	(BiP)
0.000	0.00e+00	27		3e-02	2.85e+09	862	AmorphousPocket	(I)
5.772006e-03	1.00e+00	27		1e-03	2.07e+09	1180	AmorphousPocket	(V)
0.000	0.00e+00	27		2e-03	2.43e+09	1030	AmorphousPocket	(IV)
3.254430e-04	1.29e+07	720		8e-04	1.36e+08	1130	Void	
2.241841e-03	1.04e+07	950		1	here		ThreeOneOne	
0.000	1.04e+06	27		5111	here		ImpurityCluster	(AsI)
7.615	1.40e+06	27		599	here		ImpurityCluster	(AsV)
7.573	1.40e+06	27		5228	here		ImpurityCluster	(As)
1.154401e-02	6.00e+00	27		2	here		ImpurityCluster	(BI)
17.278	4.97e+06	27		7e-04	5.66e+07	1070	ImpurityCluster	(B)
0.000	0.00e+00	27		1464	here		Elements emitting	I
0.000	0.00e+00	27		1464	here		Elements emitting	V
3.300695e-04	1.29e+07	730		936	here		Elements emitting	As
7.478722e-04	6.83e+07	1080		1e-03	2.15e+09	1130	Elements emitting	Asi
47.284	2.31e+06	27		7e-04	6.21e+07	1110	amorphous	(Recryst.)
0.000	0.00e+00	27		23025	here		LatticeAtom	

The report contains two columns with three subcolumns each. The first report shows when the model was first used; the last report shows when the model was last used. If the model is still being used, the number of particles or defects using it is displayed followed by `here`. The three subcolumns report the time, the number of simulated events, and the temperature.

For example, the previous report shows the first {311} defect (ThreeOneOne) was formed at  $2.2 \times 10^{-3}$  s, with a temperature of 950°C, and with one {311} still in the simulation. There was amorphous silicon, from 47 s, 27°C to  $6.7 \times 10^{-4}$  s at 1110°C. Since any anneal resets the time to zero, the first time applies to a previous anneal or implantation (since there is damage accumulation, in other words, room temperature annealing, during implantations).

For the interface models, the report shows how many interfaces are in the simulation (*I* and *V*), and how many of them contain trapped dopants (936 for As). It also lists the first time and the last time the interfaces let As go in the form of  $\text{As}_i$ .

This information shows how the different models were used during the simulation and when the damage was annealed.

---

## Interactions Report

This reports shows, for each material and interface, all the reactions between a mobile particle (point defect or impurity-pair point defect) and the number of times they happened.

The first column lists the name of the interacting defect, the second lists the interaction itself, and the third column lists the number of times it happened from the beginning of the simulation. Columns 4, 5, 6, and 7 are the same as 2 and 3. This report explains which reactions might be important and which are not.

For example, in the report in [PointDefect on page 526](#), the reaction I+VP (31 times) is negligible, compared to the reaction I+V (111848 times), and does not play a significant role in this simulation for the formation of APs.

Finally, depending on the defect reported, the output can differ slightly.

### PointDefect

KMC interactions report						
	Reaction	#Times	Reaction	#Times	Reaction	#Times
Silicon ---						
PointDefect	I+I	278778	I+V	111848	I+As	1435719
PointDefect	I+B	644803	I+IM	862	I+IP	7856
PointDefect	I+VMM	83	I+VM	3316	I+VP	31
PointDefect	I+AsV	273	I+AsVP	2480	I+AsVM	35
PointDefect	I+Bi	2809				
PointDefect	V+V	56907	V+As	25324	V+IM	103
PointDefect	V+IP	3541	V+VMM	288	V+VM	4248
PointDefect	V+VP	77	V+Asi	12480	V+AsiP	3405
PointDefect	V+Bi	433	V+BiP	1924	V+BiM	44
PointDefect	As+As	243	As+IM	1313602	As+VMM	38966
PointDefect	As+VM	30332	As+AsVM	2666		
PointDefect	B+IP	285066	B+BiP	203		

It includes the reaction between two mobile particles.

## Indirect Diffusion

When using the indirect diffusion model for amorphous materials, the results are similar to crystalline ones, but *I* and *V* mean *dangling bond* and *floating bond*, respectively.

	Reaction	#Times	Reaction	#Times	Reaction	#Times
--- AmorphousSilicon ---						
PointDefect	I+V	40475	I+B	30707		

## AmorphousPocket

AmorphousPocket Ix+I	713391	Ix+V	210933	Ix+VMM	305
AmorphousPocket Ix+VM	4575	Ix+VP	25		
AmorphousPocket Vx+I	31202	Vx+V	43040	Vx+IM	126
AmorphousPocket Vx+IP	11372	Vx+Bi	1281	Vx+BiM	47
AmorphousPocket IxVy+I	312602	IxVy+V	910338	IxVy+B	204
AmorphousPocket IxVy+IM	154	IxVy+IP	15555	IxVy+VMM	110
AmorphousPocket IxVy+VM	4930	IxVy+VP	5	IxVy+Bi	4683
AmorphousPocket IxVy+BiP	618	IxVy+BiM	106		

It includes the reaction between small interstitial clusters (*Ix*), small vacancy clusters (*Vx*), and APs including both *I*s and *V*s (*IxVy*). To keep the report small, all sizes are condensed into only one *Ix*, *Vx*, or *IxVy*.

## ThreeOneOne

ThreeOneOne Ix+I 1035217

All the {311} sizes are condensed under the term *Ix*.

## Loop

Loop Ix+I 177885 Ix+BiM 10

All the dislocation loop sizes are written under the term *Ix*.

## ImpurityCluster

ImpurityCluster B2+I	31	B2+Bi	6		
ImpurityCluster B3+I	3				
ImpurityCluster B2I+I	463	B2I+V	25	B2I+Bi	21
ImpurityCluster B3I+I	27591	B3I+V	1148		
ImpurityCluster BI2+V	3835	BI2+Bi	278		
ImpurityCluster B2I2+I	1518	B2I2+V	86	B2I2+Bi	1314
ImpurityCluster B3I2+I	26				
ImpurityCluster B2I3+V	26				

## 5: Atomistic Kinetic Monte Carlo Diffusion Reports

ImpurityCluster As2+V	1728	As2+As	5	As2+AsV	1251
ImpurityCluster As3+V	100	As3+AsV	69		
ImpurityCluster As4+V	3				
ImpurityCluster As2V+I	56605	As2V+Asi	20411		
ImpurityCluster As3V+I	87723	As3V+Asi	18437		
ImpurityCluster As4V+I	1973488				

Since impurity clusters are important for the correct activation and deactivation of dopants, and their sizes are small numbers, all are written in the report.

## Interface

--- Oxide_Silicon ---					
Interface	I	11364	I+As	73	V
Interface	AsV	410	Asi	1440	

The name of each particle interacting with any interface, and the number of times it happened, is reported last.

---

## Event Report

The event report is the reverse of the reaction report. The reaction report shows the forward reactions; the events report shows the reverse ones. Since the reactions and other events depend strongly on the defects, this report changes from defect to defect.

## PointDefect

KMC event report					
	Name	Jump X	Jump Y	Jump Z	Break-up
PointDefect	I	2921360317	2921305233	2921406601	
PointDefect	V	1285293026	1285290404	1285265687	
PointDefect	As	1120	1071	1163	
PointDefect	B	7	23	15	
PointDefect	IM	228653836	228646801	228625103	
PointDefect	IP	1074734274	1074760443	1074719693	
PointDefect	VMM	86102860	86115025	86090069	
PointDefect	VM	846251937	846307626	846269323	
PointDefect	VP	7881794	7875672	7878359	
PointDefect	Asi	1144728	1144688	1142864	832840
PointDefect	AsiP	51512	52143	51812	1894402
PointDefect	AsV	18255	17863	17967	30572
PointDefect	AsVP	3544	3436	3438	22783
PointDefect	AsVM	3585	3586	3460	37804

PointDefect	Bi	13459181	13453297	13458878	257929
PointDefect	BiP	94930	95115	95524	
PointDefect	BiM	124899	123825	124860	670411

The second column shows the name of the mobile particle. The 3rd, 4th, and 5th columns show how many diffusion events (hops or jumps) have every particle perform in the x-, y-, and z-axis, respectively. In the absence of anisotropies, these three numbers must be approximately the same. Finally, the last column shows the number of breakups. Since not all the mobile particles can break up (for example,  $B_i$  will break in  $B + I$ , but  $I$  cannot break up), some particles will have an empty column. The relative number between the number of diffusion steps and the number of breakups gives an estimation of the stability of the particle. The more stable the particle (more diffusion events and fewer breakups), the larger its long-hop distance.

When using the double-hop model, the report looks like:

	Name	Jump <>	Jump >>	Jump > <sup>^</sup>	Break-up
PointDefect	I	288583696	288599278	1154233402	
PointDefect	V	524892	527369	2103188	
PointDefect	IM	32935856	32946513	131772254	
PointDefect	IP	153307399	153285675	613169175	
PointDefect	VMM	373744	374963	1498954	
PointDefect	VM	256003	255776	1022437	
PointDefect	VP	309	260	1111	
PointDefect	VPP	4	4	10	
PointDefect	AsV	14570	14473	58109	47289
PointDefect	AsVM				223313
PointDefect	AsVP	348	371	1464	3547
PointDefect	Asi	102330	102738	411863	839856
PointDefect	AsiP	8695	8669	34730	843920
PointDefect	BV	41	30	157	3
PointDefect	BVM	166	181	682	280
PointDefect	BVP				1
PointDefect	Bi	26231	25952	104499	21468
PointDefect	BiM	9798	9735	39016	42747

In this report, the third column reports the number of jumps in opposite directions. The fourth column reports the number of jumps in the same direction, and the fifth column lists jumps in orthogonal directions. For further information, see [Hopping Mode on page 417](#).

## AmorphousPocket

	Name	IV Recom	I Emis	V Emis
AmorphousPocket	Ix		300905	
AmorphousPocket	Vx			59627
AmorphousPocket	IxVy	802007		

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Reports

$I_x$  are small interstitial clusters. They can only emit interstitials.  $V_x$  are small vacancy clusters that can only emit vacancies. Finally,  $I_x V_y$  are APs. They can recombine (destroy) an internal IV pair.

### ThreeOneOne

	Name	I Emis
ThreeOneOne	$I_x$	1038899

{311}s can only emit neutral interstitials.

### Loop

	Name	I Emis
Loop	$I_x$	181927

Dislocation loops, like the {311}s, can only emit neutral interstitials.

### ImpurityCluster

Name	Emis
ImpurityCluster B3	10 V
ImpurityCluster B3I3	913 I 14203 Bi
ImpurityCluster B2I3	4710 I
ImpurityCluster B3I2	13570 I
ImpurityCluster B2I2	656 I
ImpurityCluster BI2	1 I 32 Bi
ImpurityCluster B2I	578 BiP

An impurity cluster (for example, a BIC) emits  $B_i$  and  $I$ .  $B_2I$  also can emit  $B_iP$  particles. Finally, an internal Frenkel pair can be created, trapping the  $I$  and emitting the  $V$ . This has been the case in this simulation for 10  $B_3$  ( $B_3 \rightarrow B_3I + V$ ). Since  $BV$  is not defined by default, it cannot be emitted.

Name	Emis
ImpurityCluster B3	1 V
ImpurityCluster B2	10 V
ImpurityCluster B3I2	6 I
ImpurityCluster C2I	3 I 1 V 32 Ci
ImpurityCluster B3I	1 V 6 Bi
ImpurityCluster B2I	107 Bi
ImpurityCluster CB2I	84 Bi 2 Ci
ImpurityCluster CBI	42 I 1 Bi

In this case, apart from more or less standard boron and carbon clusters, there is a hypothetical carbon–boron–interstitial (CBI) cluster. Two members of this CBI cluster are present here,  $\text{CB}_2\text{I}$ , emitting  $\text{B}_i$  and  $\text{C}_i$ , and CBI, emitting I and  $\text{B}_i$ .

## Amorphous Defects

	Name	Recryst.		
Amorphous	Ele.	4932 B <sub>3</sub> I <sub>3</sub>	4598 B <sub>2</sub> I <sub>3</sub>	7087 BI <sub>2</sub>

This is an example of recrystallization of depositing inactive boron in different cluster configurations. In this case, the simulator tries to deposit the impurity clusters with a proportion of 30%, 30%, and 40% for  $\text{B}_3\text{I}_3$ ,  $\text{B}_2\text{I}_3$ , and  $\text{BI}_2$ , respectively.

## Lattice Atoms

	Name	SPER	
LatticeAtom	I	2070434	

Example of output related with epitaxial growth, showing the number of atoms that were incorporated into crystalline silicon.

## Simple Materials

An event report is written for simple materials as well:

--- AmorphousSilicon ---					
	Name	Jump <	Jump >>	Jump >^	Break-up
PointDefect	B	4	2	16	
amorphous	Name	Recryst.			
	I	7575			
Rejected PD	Name	Jump <	Jump >>	Jump >^	
	As		9	42	

## Indirect Diffusion

The report for amorphous materials with indirect diffusion is similar to the one of crystalline materials, but the *I* and *V* mean *dangling bond* and *floating bond*, respectively.

--- AmorphousSilicon ---					
	Name	Jump <	Jump >>	Jump >^	Break-up
PointDefect	I	408765	409824	1637334	
PointDefect	V	244177	244724	975635	
PointDefect	Bi	456685	457074	1824373	30707
	Name	Jump <	Jump >>	Jump >^	

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Extracting KMC-Related Information

Rejected PD	I	141130
Rejected PD	V	85422
Rejected PD	Bi	155922

---

## Extracting KMC-Related Information

You can extract Sentaurus Process KMC information in one of the following ways:

- Using the Sentaurus Process interface (in some cases, the information must be translated to Sentaurus Process fields using the `kmc deatomize` command before calling the Sentaurus Process commands):
  - The `struct` command
  - With the `select`, `print`, `WritePlx`, and `plot` commands
- Calling directly the Sentaurus Process KMC kernel:
  - Writing Sentaurus Process KMC TDR files
  - Extracting atomistic information with the `kmc extract` command (see [kmc on page 1037](#))

Calling Sentaurus Process KMC directly has the following advantages:

- More information can be obtained than using the regular interface.
- The atomistic continuum conversions needed to compute the concentrations are more accurate.
- The atomistic information (that is, 3D coordinates and the defect shapes) can be displayed.
- Simulations can be saved and reloaded.

---

## Transferring Fields From KMC to Continuum Information: `deatomize`

Sentaurus Process KMC is independent of the mesh and fields of Sentaurus Process. Consequently, after a diffusion in atomistic mode, there are no Sentaurus Process fields to visualize. You can instruct Sentaurus Process KMC to create fields with KMC information. For example, to deatomize the simulation and convert the 3D positions into concentrations, use:

```
kmc deatomize name=<c>
```

When the field is created, Sentaurus Process KMC will not modify it unless there is a new `kmc deatomize` command.

This means that the field is synchronized with the Sentaurus Process KMC simulation when it is created. However, after that, if the simulation changes (for example, performing another diffusion), the field will conserve the initial values.

The fields created by the `kmc deatomize` command are:

- Concentration of particles (number of particles per volume unit). It could be substitutional (`B`, `As`, ...), paired (`ASV`, `Bi`), and the charge state is included (`ASV` is neutral; `ASVM` is negative). If these particles are mapped as *mobile* in the `KMC.tcl` file (see [Including New Impurities on page 518](#)), the field will be computed as an average of time. Otherwise, the field will contain the instantaneous concentration.
- Total concentration of impurities (number of particles in any defect per volume unit): `Itotal`, `BTOTAL`, ...
- Concentration in the interface (number of particles in the interface per volume unit): `BInterface`, `AsInterface`...
- Concentration in amorphous material (number of particles in amorphous layers per volume unit): `AsAmorphous`, `BAmorphous`...
- Concentration of a particular extended defect (number of defects, where one defect contains more than one particle, per volume unit): `I54`, `V23`, `I1026`...
- Concentration of a particular AP (number of APs, where an AP contains more than one particle): `IV`, `I3V4`...
- Concentration of a particular impurity cluster (number of impurity clusters, where an impurity cluster contains more than one particle): `B2I3`, `As4V`...
- Active concentrations (active number of dopants per volume unit, net, p-type, n-type, and total): `NetActive`, `pNetActive`, `nNetActive`, `tNetActive`.
- Germanium concentration: `Ge`.

Some fields compute the defect concentration (concentration of APs, impurity clusters, and extended defects). To transform them into particle concentrations, multiply by the size of the defect.

For example, you can obtain the concentration of boron particles in  $B_2$ ,  $B_3$ ,  $BI_2$ , and  $B_2I_2$  in the field BICs with the following commands:

```

kmc deatomize name= B2
kmc deatomize name= B3
kmc deatomize name= BI2
kmc deatomize name= B2I2
select z= "2*B2 + 3*B3 + BI2 + 2*B2I2" name= BICs

```

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Extracting KMC-Related Information

## Smoothing Out Deatomized Concentrations

The direct deatomization of Sentaurus Process KMC quantities into continuum mesh elements produces values with strong gradients between neighboring elements. This is especially true for small concentrations, where Sentaurus Process KMC contains a few particles that are deatomized as an ‘all or nothing’ distribution; that is, some cells may contain one particle, and this is a concentration of  $1/(\Delta V)$ , while others contain no particles, thereby having a zero concentration.

In some cases, especially when the Sentaurus Process KMC output is used as a device simulation input, a smoother concentration is needed, as seen in [Figure 65](#). This can be performed by setting the parameter `Smooth.Field`:

```
pdbSet KMC Smooth.Field <field> <n>
```

where:

- `<field>` is the field name to be smoothed (for example, `NetActive`).
- `<n>` is an integer.

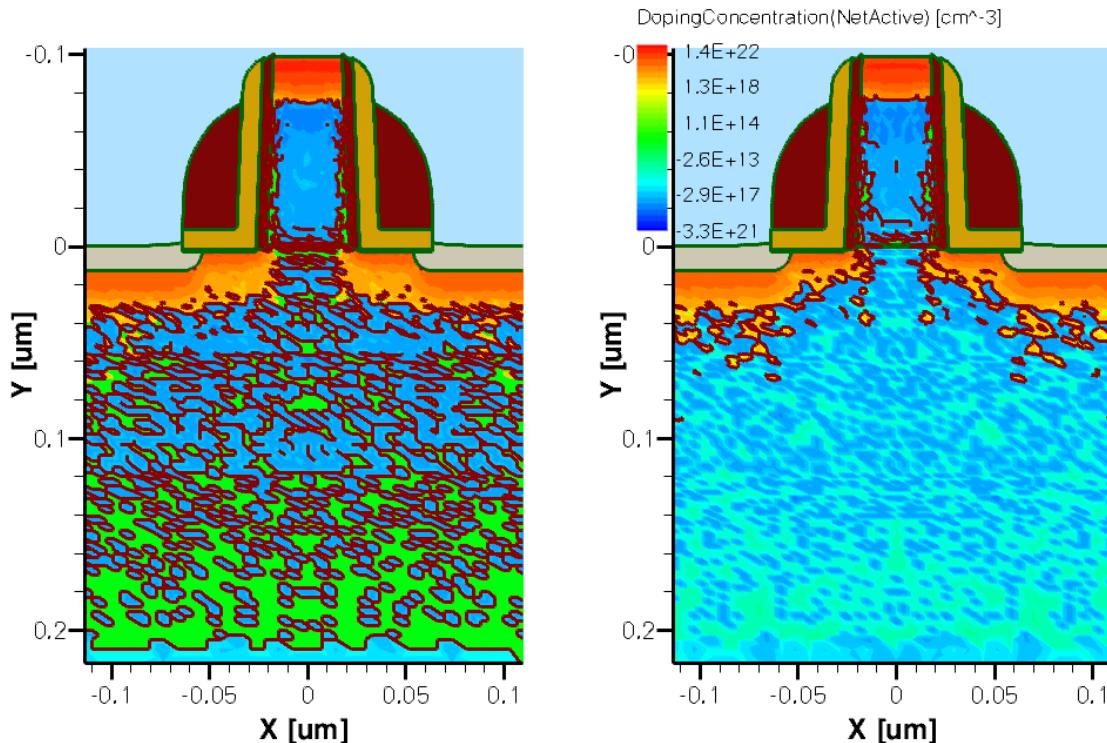


Figure 65 Comparison of NetActive concentration in simulations performed with (*left*) `Smooth.Field` set to 0 (disabled) and (*right*) `Smooth.Field` set to 1

A value of 0 produces no smoothing; larger numbers produce more smoothed profiles. The smoothing algorithm works as follows:

- For each node in the standard Sentaurus Process mesh, the number of particles  $N$  associated with the node is counted.
- The concentration set to that node is, in principle,  $N/V^{\text{Voronoi}}$ , where  $V^{\text{Voronoi}}$  is the Voronoï volume associated with the node.
- $N$  is compared to  $M$ , where  $M$  is the value specified in `Smooth.Field` for this field.
- If the field name does not exist in `Smooth.Field`, 0 is assumed.
- If  $N < M$ , the smoothing algorithm applies. Starting at the node, the algorithm looks for particles not associated with the Voronoï volume of the node, with an increasing radius.
- When  $M - N$  particles are found in a radius  $R$ , it stops searching. At this point, there are  $M$  particles inside the radius,  $M - N$  outside the Voronoï volume, and  $N$  inside the Voronoï volume.
- Then, the concentration of the node will be:

$$N/V^{\text{Voronoi}} + \frac{\text{weight} \times (M - N)}{V_R} \quad (839)$$

where  $V_R$  is the volume associated with a segment (1D), circle (2D), or circumference (3D) of radius  $R$ , and `weight` is the PDB value `Smooth.Weight`:

```
pdbSet KMC Smooth.Weight 0.01
```

This technique is not intended to perfectly conserve the total dose, but to fill the nodes with low concentrations with values depending on the distance to the nearest particles. The factor `weight` is included to limit the extra dose introduced in those nodes.

The `Smooth.Field` parameter is used whenever a deatomization is performed. This includes calling directly `kmc deatomize` from the command line or indirectly through the `KMC2PDE` procedure or another procedure.

## Smoothing Performance

The smoothing algorithm can be relatively slow for simulations with a large number of nodes or particles. Using parallel mode with the following command may help improve performance:

```
math numThreadsDeatomize=<i>
```

For extreme cases with very large meshes, smoothing may be too slow to be useful even in parallel mode. To disable it completely, use:

```
pdbSet Smooth.Field {}
```

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Extracting KMC-Related Information

This option is independent of the KMC parallel mode and does not interfere with it. It applies to the smoothing algorithm only, not to the whole deatomization.

---

## Adding and Obtaining Defects in Simulations: `add`, `defects.add`, and `defects.write`

Sentaurus Process KMC allows you to add defects to a simulation using the commands:

```
kmc add queue name=<c> coordx=<n> coordy=<n> coordz=<n> [amorphous]  
[crystalline]  
kmc add
```

First, the defects are added to the creation queue with the command:

```
kmc add queue
```

You can queue as many defects as you want. Queueing a defect does not actually introduce it in the simulation. You must use the command `kmc add` alone to empty all of the queue by generating defects in the simulation.

The `name` argument specifies the defect to be created (for example, `B`, `B2I4`, `I54`, and `BInterface`). The `coordx`, `coordy`, and `coordz` arguments specify the place where the defect (or the center of mass of the defect) will be created. The options `amorphous` and `crystalline` specify whether this defect should be created in an amorphous or a crystalline material. For example, if the current material is crystalline, but `amorphous` is specified, the simulator not only creates a defect, but also changes the material from crystalline to amorphous phase.

Alternatively, to add defects to the simulation, use the `defects.read` argument, which specifies the name of a text file from which to read its defects, for example:

```
kmc defects.read= my_filename
```

This command takes all the defects specified in the file and adds them consecutively in a very similar way to the `kmc add` command. Similar to the `kmc add` command, only the center of mass is specified for defects having more than one particle.

One line specifies one defect. The format of each line is:

```
defect_type defect_name coord_x coord_y coord_z
```

where:

- `defect_type` is the generic name of the defect, for example, `PointDefect`, `Loop`, `ThreeOneOne`, `Interface`, `ImpurityCluster`.

- `defect_name` is the particular name of the defect, for example, `B`, `P`, `I50`, `BiM`, `B3I2`.
- `coord_x`, `coord_y`, `coord_z` are the coordinates (in nanometers) of the center of mass of the defect.

For example:

Interface	P	1.000000	11.250000	13.000000
PointDefect	As	5.032000	5.320000	1.032000
ThreeOneOne	I50	10.000000	10.222565	9.777436
PointDefect	B	10.000000	5.000000	6.000000
PointDefect	BiM	30.000002	5.000000	14.000000
ThreeOneOne	I100	19.554871	20.445129	20.000000
Loop	PI59	13.000000	13.000000	13.000000
PointDefect	Bi	26.000000	26.000000	26.000000
ImpurityCluster	B2I	6.235641	7.115777	7.077633
ImpurityCluster	B3I2	4.287220	7.497602	4.604665
PointDefect	Ge	6.696747	7.492962	0.834044

Similarly, to write all the defects currently in the simulation into a file with the above format, specify the name of the file:

```
kmc defects.write= my_filename
```

Files written with `defects.write` can be read later with `defects.read`. Since only the center of mass of the particle is written, this is an inaccurate way to save a simulation.

To save a simulation, use instead the `struct` command or the `kmc extract tdrWrite` command.

## Updating a KMC Structure in Nonatomistic Mode

When working in hybrid mode, the Sentaurus Process KMC structure is not updated automatically when required. For example, during an `etch` step or a `strip` step, if a region containing particles has been removed, the particle information is not removed until the Sentaurus Process KMC structure is updated.

You should specifically call `kmc remesh` to update the Sentaurus Process KMC structure, immediately after the step. This call ensures that any defects or particles in the region that have been removed are also removed from the Sentaurus Process KMC structure. The structure update would not occur unless the continuum structure has changed as well. In this way, unnecessary time spent in remeshing is avoided.

---

## Using the Sentaurus Process Interface

### The select, print, WritePlx, and plot Commands

The commands `select`, `print`, `WritePlx`, and `plot` work as expected. If you need a field for them, create it using the `kmc deatomize` command (see [Transferring Fields From KMC to Continuum Information: deatomize on page 532](#)).

In particular, the `select` command creates particles inside Sentaurus Process KMC whenever the name of the field is recognized as a particle or defect. These names are:

Dopants	As, B, ...
Impurities	C, F, ...
Paired particles	Bi, AsV, Ci, ...
Point defects	I, V
Any of the above particles with a different charge	IM, VPP, BiM, AsVP, ...
Amorphous	BAmorphous, AsAmorphous, ...
Amorphous pockets	IV, I4V5, ...
Dopants or impurities in an interface	BInterface, AsInterface, ...
Extended defects	I43, V21, ...
Impurity clusters	AsV4, BI2, ...

### Examples

For a typical situation with a 1D SIMS-like simulation (implantation and anneal), the 1D profiles can be extracted to a `.plx` file using `WritePlx`:

```
SetPlxList BTotal B  
WritePlx file
```

Calling `WritePlx` without selecting the list with `SetPlxList` also works. It generates a list of the most common fields:

```
WritePlx file
```

In nonatomic mode, the fields must be deatomized first:

```
kmc deatomize name=BTotal  
kmc deatomize name=B
```

## The init Command

The `init` command works as expected. Background dopings can be assigned. A TDR file to be loaded can also be assigned with:

```
init tdr=<c>
```

If the file has been saved with Sentaurus Process KMC and contains atomistic information (see the option `defects` for `tdrAdd`; [kmc on page 1037](#)), Sentaurus Process will load it, and the simulation can continue.

**NOTE** Loading a file and continuing a simulation with the `init` command will give results similar, but not identical, to performing the simulation without the save/load process. The differences between the results are only statistical, that is, both represent possible solutions.

## The struct Command

The `struct` command works as expected, except that by default it creates some extra fields to be saved. It generates these extra fields by calling the function `PDE2KMC` with the argument `struct`. You can modify or customize this function in the `KMC.tcl` file. By default, `PDE2KMC` tries to generate and store fields similar to a five-stream model from the KMC information.

The `struct` command also saves restart information, allowing the Sentaurus Workbench `#split` command to work properly with Sentaurus Process KMC.

## The load Command

The `load` command accepts the options `kmc` and `replace` only. It is intended to load a TDR Sentaurus Process KMC simulation to replace the existing one. It performs the necessary conversions between the existing internal Sentaurus Process KMC and the one read from the TDR file, conserving the existing one.

## The deposit Command

The `deposit` command works as expected, including depositing doped layers.

## The diffuse Command

The `diffuse` command works as expected with Sentaurus Process KMC, except that the diffusion is performed with the atomistic solver. In particular, the options for oxidation and silicidation are supported (see [Oxidation on page 517](#)). Epitaxial options also are supported.

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Extracting KMC-Related Information

For lattice LKMC epitaxy, see [Chapter 6 on page 567](#).

## Nonatomistic Mode

When Sentaurus Process KMC operates in nonatomistic mode (see [Nonatomistic Mode on page 378](#)), it transforms the five-stream model fields into atomistic information before every annealing and converts the atomistic information to five-stream model information after any annealing. Sentaurus Process KMC is disabled between annealings; consequently, all information should be accessed using the standard Sentaurus Process interface. The only way to access atomistic information is to use the `Movie` option during the Sentaurus Process KMC annealings.

The transformation from five-stream to atomistic information is performed in the function `PDE2KMC` with the argument `diffuse` in the `KMC.tcl` file. The function `PDE2KMC` is called automatically before a Sentaurus Process KMC diffusion in nonatomistic mode. After the diffusion, the function `KMC2PDE`, with argument `diffuse`, is invoked to convert the atomistic information into five-stream fields. You can modify and customize both functions.

## Atomistic Mode

When operating in atomistic mode, Sentaurus Process KMC does not automatically perform any transformation from atomistic to continuum, or vice versa, except if the `struct` command is called (see [Atomistic Mode on page 375](#)).

---

## Calling Directly the Sentaurus Process KMC Kernel

The best way to access atomistic information is by calling directly the Sentaurus Process KMC kernel using the `kmc extract` command, which accesses the raw KMC information directly and returns it in different formats, or creates a TDR file to be opened with Sentaurus Visual.

## Writing and Displaying TDR Files With KMC Information

To write all snapshots to a file to be displayed by Sentaurus Visual, use:

```
kmc extract tdrWrite filename=<c>
```

Each snapshot is taken at a particular time during the simulation. The collection of snapshots provides information about the time evolution during the simulation. Each snapshot can contain concentrations and histograms, atomistic information, or both.

These snapshots must first be created with the command:

```
kmc extract tdrAdd [concentrations] [defects] [Stress] [histogram]  
[visual= <list>] [list= <list>]
```

The option `concentrations` includes a list of standard fields. These fields are the total concentration for each particle, the time-averaged concentrations of mobile particles, `NetActive`, the electronic concentration, the concentration of impurities in the surface, amorphous and impurity clusters, and the concentration of point defects in APs, amorphous layers, impurity clusters, and extended defects. These concentrations are displayed with the same dimension as the simulation.

Since Sentaurus Process KMC always works in three dimensions, for 1D simulations, the displayed concentrations are averaged for  $yz$  planes and, for 2D simulations, they are averaged in  $z$ -lines. An extra `A/C` field also is stored to let you know whether the material is amorphous or crystalline.

The `histogram` option includes a 2D graph representing the APs and impurity-cluster histograms. These histograms give the number of defects existing in the simulation for each different size ( $I$  and  $V$  for APs, impurities, and point defects for impurity clusters). One-dimensional histograms, giving the number of extended defects versus its size, are included as well when using the `histogram` option. Stress and strain information can be added to these concentrations and histograms with the `Stress` option.

[Figure 66 on page 542](#) shows the visualization of a TDR file saved with the `concentrations` and `histogram` options for a 2D simulation. The `concentrations` option allows the concentration of several fields to be included in a TDR file.

Regarding `NetActive`, the parameter `KMC tdr smoothDopingConcentration` controls whether this concentration is smoothed. By default, it is not smoothed because smoothing it artificially decreases the channel length. On the other hand, the smoothing algorithm partially removes irregularities and other atomistic features that may appear on the p-n junctions. This smoothing differs from the one controlled by `Smooth.Field` (see [Smoothing Out Deatomized Concentrations on page 534](#)).

While `smoothDopingConcentration` controls the smoothing of only `NetActive` in the Sentaurus Process KMC TDR file, `Smooth.Field` controls the smoothing of any field when translating atomistic information into the continuum mesh concentration.

The option `defects` includes atomistic information about the defects in the simulation. This atomistic information can be used to obtain an atomistic 3D plot that is independent of the simulation dimensions. It offers the most realistic representation of the simulation.

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Extracting KMC-Related Information

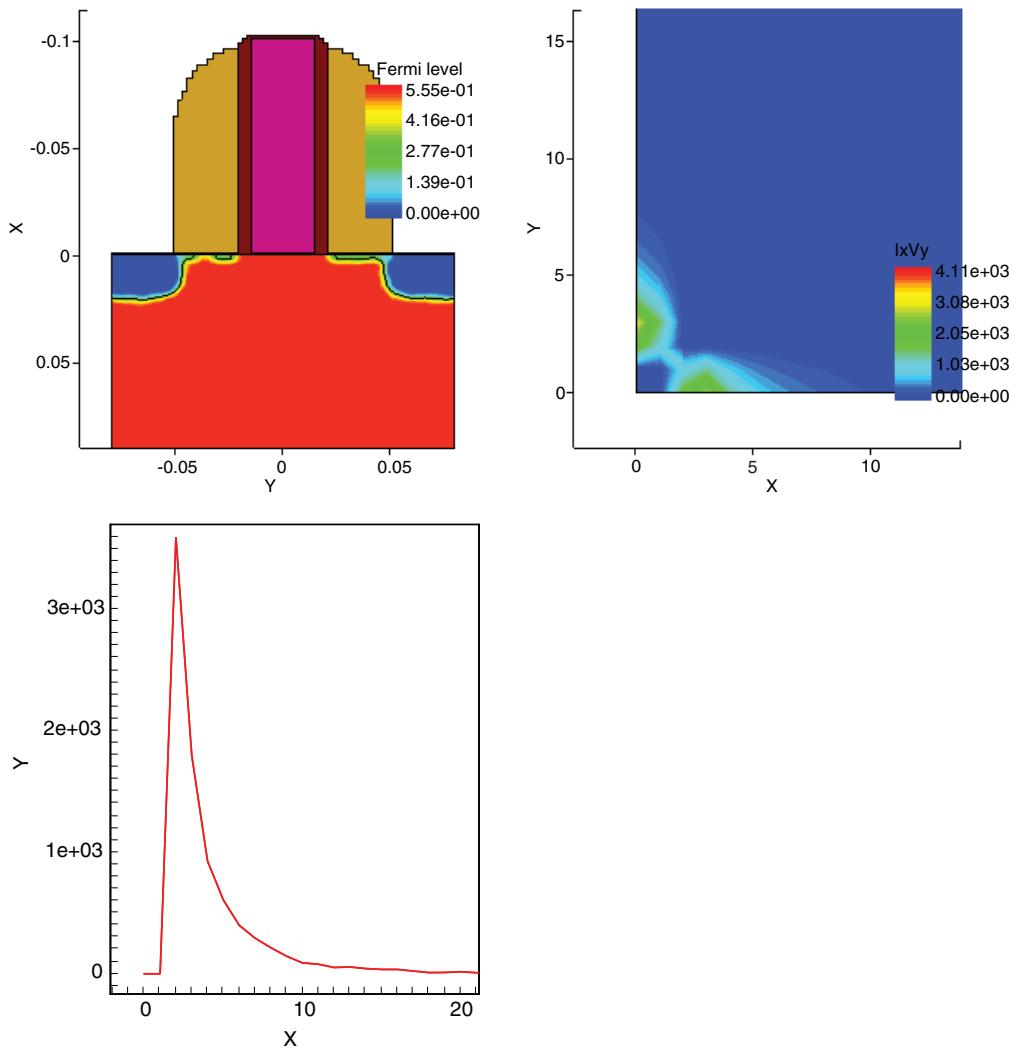


Figure 66 Visualization of a TDR file saved with the concentrations and histogram options: (upper left) 2D representation of Fermi level concentration, (upper right) 2D histogram of amorphous pockets and dopant clusters, and (lower left) histogram for clusters

Figure 67 shows an example of information saved with the `defects` option.

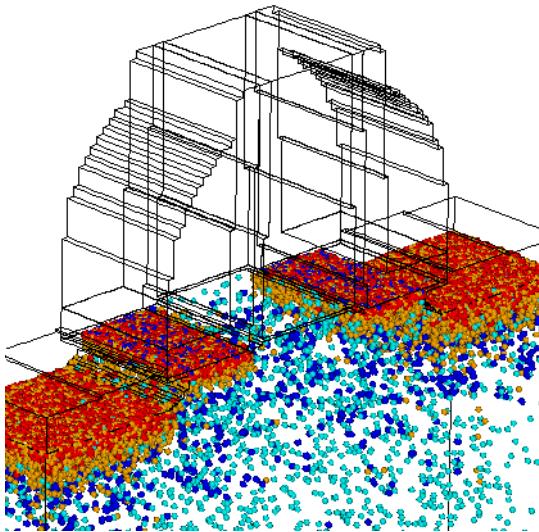


Figure 67 Visualization of individual defects of a 3D MOSFET device simulated by Sentaurus Process KMC

The `defects` option also includes extra information necessary to restart or load the simulation. A file saved with this option can be reloaded into Sentaurus Process KMC, and the simulation can continue. To load the simulation, use the `init` command.

Using the `KMC Movie` option, you can include the `kmc extract tdrAdd` command to view the evolution of the simulation with time.

Finally, the option `visual` stores atomistic 3D information in a way similar to the `defects` option. The differences between using `visual` and `defects` are:

- Files saved with `visual` cannot be restarted.
- The `visual` option produces smaller file sizes than `defects`. In particular, `visual` stores the defects, but it does not store the information needed to restart the simulation. The `visual` files are intended for visualization purposes only.
- The `visual` option requires a list of defects, separated by commas, to be saved. To save all defects, specify `visual=all`.
- Other valid defects include defect names (such as `BiM` or `B2I3`), general defect names (such as `ThreeOneOne`), and material names (`Silicon`). This lets you control which defects will be saved and visualized later, making it easier to visualize information without saving a large file with all the 3D information.

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Extracting KMC-Related Information

#### Plotting Only Some Particles

Sentaurus Process visualization does not represent all the particles inside APs. Since the number of particles (interstitials and vacancies) in APs can be large after an implantation, only 1 in 50 particles is visualized by default. This default behavior is written in the TDR file as set by the parameter `VisualizeDamage`:

```
sprocess> pdbGet KMC VisualizeDamage  
50
```

Sentaurus Process visualization can overwrite the default set for each file using the option:

```
-s:psf n
```

where `n` is the new value of `VisualizeDamage`.

**NOTE** Setting `VisualizeDamage 1` causes Sentaurus Visual to plot all the particles present in the simulation. This number can be very large immediately after an implantation.

#### Time-Averaged Concentration Name

The default field name for time-averaged concentrations in the TDR file is ‘mobile’, but it can be defined with the parameter `pdbSet KMC tdr averageTag`.

---

## Extracting KMC Profiles, Histograms, and Defects

Besides the `select` command and TDR files, you can extract Sentaurus Process KMC information using the `kmc extract` command (see [kmc on page 1037](#)) including:

- `kmc extract histogram` extracts histograms for extended defects, impurity defects, and APs.
- `kmc extract profile` extracts concentrations and stresses in 1D, 2D, and 3D.
- `kmc extract supersaturation` extracts the concentration relative to the equilibrium concentration for point defects.
- `kmc extract defects` obtains the atomistic information of the defects.
- `kmc extract dose` extracts doses, that is, concentrations in  $\text{cm}^{-2}$ .
- `kmc extract materials` obtains information about the different materials in the simulation.
- `kmc extract acinterface` obtains the positions of the amorphous-crystalline interfaces in the simulation.

## Extracting Histogram Information

Use the command:

```
kmc extract histogram name=<c> [meansize [minsize=<n>]] [materialname=<c>]
```

Sentaurus Process KMC includes several models where the defects are not isolated, but agglomerated in extended defects that can contain many particles. The `histogram` option allows you to extract information about the sizes (number of particles) of these extended defects.

You must specify a valid name to compute the following available histograms:

Interstitial-extended defects      `name=I` extracts information about small I clusters, {311} defects, and dislocation loops.

Vacancy-extended defects      `name=V` extracts information about small V clusters and voids.

B interstitial clusters or `name=XI` extracts information about the dopant named x. For other clusters with I example, for boron impurity clusters (BICs), `name=BI`.

As vacancy clusters or `name=XV`. For example, set `name=ASV` to extract information about arsenic–vacancy clusters.

Cluster with multiple impurities      For example, set `name=PAs` for clusters with both P and As.

Amorphous pockets      `name=IV` extracts information about APs.

Use the optional `meansize` to display the average size of clusters instead of the whole list of clusters. Without specifying `minsize`, the average size begins with size 0.

The `materialname` argument restricts the output to the material specified instead of the entire simulation.

### Interstitial Histograms

These histograms extract the number of defects in the simulation for each size. The histograms contain information about small irregular clusters (see [Amorphous Pockets Life Cycle on page 434](#)), {311} defects (for sizes bigger than the established limit), and dislocation loops.

For example:

```
LogFile [kmc extract histogram name=I]
```

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Extracting KMC-Related Information

returns a list of extended defects with  $I$ :

```
sprocess> LogFile [kmc extract histogram name=I]
I2 302
I3 104
I4 42
I5 12
I6 4
I72 1
I677 1
sprocess> LogFile [kmc extract histogram name=I meansize]
4.11373
sprocess> LogFile [kmc extract histogram name=I meansize minszie=10]
374.5
```

### Vacancy-Extended Defects Histogram

These histograms are similar to the interstitial-extended defects histogram, except that the extracted number of particles versus size is for vacancies. For example:

```
sprocess> LogFile [kmc extract histogram name=V]
V5 1
V7 2
V8 5
V9 2
V10 5
(...)
sprocess> LogFile [kmc extract histogram name=V meansize]
12.9143
sprocess> LogFile [kmc extract histogram name=V meansize minszie=10]
15
```

### Amorphous Pockets Histogram

The AP histograms contain the number of cluster versus  $I$  and  $V$  size. APs with null  $I$ s or  $V$ s can be considered as APs or small  $I$  or  $V$  clusters. For example:

```
sprocess> LogFile [kmc extract histogram name=IV]
I2 367
I3 69
I4 22
I5 1
IV 823
I2V 249
I3V 61
I4V 23
I5V 2
V2 408
IV2 251
```

```
I2V2 111  
(...)
```

The average size can be requested for these clusters. It will return values for both *I* and *V*:

```
sprocess> LogFile [kmc extract histogram name=IV meansize]  
I2.3501V0.796781
```

The parameter `meansize` specifies the minimum size to begin the average for both species.

### Boron–Interstitial Clusters

The boron–interstitial cluster histogram offers information about the number of BICs for each BIC configuration ( $B_nI_m$ ):

```
sprocess> LogFile [kmc extract histogram name=BI]  
B2I 16  
B3I 347  
sprocess> LogFile [kmc extract histogram name=BI meansize]  
B2.95592I1
```

### Arsenic–Vacancy Clusters

The arsenic–vacancy cluster histogram offers information about the number of arsenic and vacancies in impurity clusters for each configuration ( $As_nI_m$ ):

```
sprocess> LogFile [kmc extract histogram name=AsV]  
As2 277  
As3 109  
As4 3  
As2V 752  
As3V 281  
As4V 178  
sprocess> LogFile [kmc extract histogram name=AsV meansize]  
As2.47V0.756875
```

## Extracting Concentrations

Sentaurus Process KMC computes the profiles concentration versus size as a convenient way to directly obtain useful data.

To extract concentrations, use:

```
kmc extract profile name=<c> [defectname=<c>] [materialname=<c>]  
[timeaveraged] [coordx=<n>] [coordy=<n>] [coordz=<n>]
```

## 5: Atomistic Kinetic Monte Carlo Diffusion

### Extracting KMC-Related Information

where name specifies the profiles to be extracted:

- electrons returns the concentration of electrons.
- holes returns the concentration of holes.
- A particle name (such as Bi, IM, or AsVP) returns the concentration of all particles in the simulation matching the given one.
- A cluster name (for example, As4V) returns the concentration of that cluster in the simulation. For example, an As<sub>4</sub> cluster is considered to be four As particles when you request the concentration of As, but only one defect when you request the concentration of As<sub>4</sub> clusters.
- stressXX, stressYY, stressZZ
- strainXX, strainYY, strainZZ, strainXY, strainYZ, strainXZ
- Bandgap, gap
- GapNarrowing returns the bandgap narrowing in eV.
- dopants
- Fermi\_level
- ni returns the intrinsic concentration.
- An impurity name followed by Total (such as BTot and AsTotal) returns the total profile of that impurity (active, inactive, in pairs, clusters and so on) in the simulation.

For example, 1D profiles can be compared with SIMS experiments. The profiles are an average of the concentration of particles. For 3D, Sentaurus Process KMC takes a volume to be averaged equal to an element defined by the parameters extractDeltaX, extractDeltaY, and extractDeltaZ. For 2D and 1D, this volume includes all the elements in y and z, respectively.

When a particle profile is specified, the optional argument defectname can be used to further specify the kind of particle (see [Table 58 on page 407](#)). For example, the following command computes the concentration of interstitials in any kind of defect, that is, the total interstitial concentration:

```
kmc extract profile name=I
```

The following command computes the concentration of interstitials in impurity clusters:

```
kmc extract profile name= I defectname= ImpurityCluster
```

**NOTE** The argument defectname must not be specified with cluster concentrations, electrons, holes, Bandgap, gap, GapNarrowing, Fermi\_level, ni, stresses, or strains.

The argument materialname restricts the output to the material specified instead of the entire simulation.

The returned concentration has the same dimensionality as the performed simulation. Use `coordx`, `coordy`, and `coordz` to change this default. These arguments specify cutlines. For example, in a 3D simulation, the following command returns the concentration for all the volume elements in the simulation:

```
kmc extract profile name=I
```

The following command returns a 1D profile with concentrations in the plane  $x = 20$  nm and  $z = 10$  nm:

```
kmc extract profile name= I coordx= 20<nm> coordz= 10<nm>
```

The following command returns only one value, the concentration at the specified point:

```
kmc extract profile name= I coordx= 20<nm> coordy= 15<nm> coordz= 10<nm>
```

The use of `coordx`, `coordy`, and `coordz` depends on the simulation dimensions. As previously explained, specifying `coordx` for 1D, 2D, or 3D simulations, `coordy` for 2D or 3D, or `coordz` for 3D, returns the concentrations only on elements including the specified cutlines. On the other hand, the use of `coordy` or `coordz` in 1D simulations, or `coordz` in 2D, is quite different. In this case, the result returned is not averaged for the whole remaining dimensions ( $y$  and  $z$  for 1D,  $z$  for 2D), but only calculated in the specified cutlines. In other words, specifying `coordy` in a 3D simulation returns all the concentrations in the  $x, z$  volumes for the  $y$  specified in `coordy`; while specifying `coordy` in a 1D simulation returns concentrations versus the  $x$ -axis, but instead of being averaged for every  $y$  and  $z$ , they will be averaged only for every  $z$  in the plane marked by `coordy`. In 3D, it will reduce the size of the output (since only the output for the specified plane  $y$  is written). In 1D, the output has the same number of lines (one for each  $x$  position), but the concentration displayed is different because it is averaged into  $z$  only, and not into  $y$  and  $z$ .

Sentaurus Process KMC returns the instantaneous concentration by default. For mobile particles, the instantaneous concentration does not usually contain any information other than noise. The option `timeaveraged` instructs Sentaurus Process KMC to return the average concentration of mobile particles between the current time and the last time Sentaurus Process KMC created a snapshot (see [Snapshots on page 399](#)).

For example, [Figure 68 on page 550](#) has been produced with the input script:

```
pdbSet KMC MaxYum 40e-3
pdbSet KMC MaxZum 40e-3
SetAtomistic
pdbSet KMC Movie ""
pdbSet IncrementalHops 0
line x loc=0.0    tag=xleft   spacing = 0.002
line x loc=1.5e-3 tag=xmed    spacing = 0.002
line x loc=5e-3   tag=xright  spacing = 0.002
```

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### Extracting KMC-Related Information

```
region oxide  xlo=xleft xhi=xmed
region silicon xlo=xmed  xhi=xright

init
diffuse time=1e7<s> temp=700 info=1
kmc extract tdrClear
kmc extract tdrAdd concentrations
kmc extract tdrWrite filename=equil
```

The concentrations of neutral, positive, and negative interstitials also can be obtained with:

```
sprocess> kmc extract profile timeaveraged name=IP coordx=2.5<nm>
162487
sprocess> kmc extract profile timeaveraged name=I coordx=2.5<nm>
1.0276e+06
sprocess> kmc extract profile timeaveraged name=IM coordx=2.5<nm>
18170.5
```

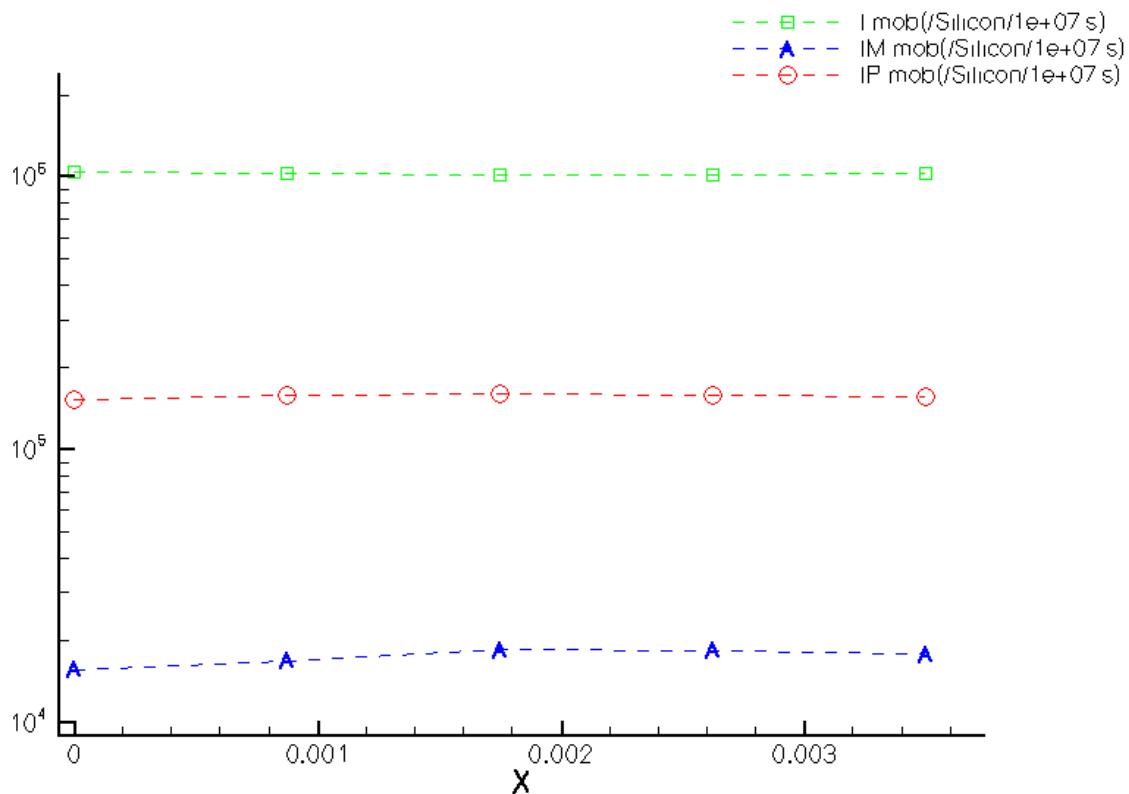


Figure 68 Equilibrium concentrations of neutral (green), positive (red), and negative (blue) interstitials at 700°C

## Extracting Supersaturation

To extract supersaturation, use:

```
kmc extract supersaturation name=<c>
```

where name can take the value I or V only.

Supersaturation is the current concentration relative to the equilibrium concentration:

$$\text{supersaturation}(X) = \frac{[X]}{[X]^*} \quad (840)$$

Sentaurus Process KMC computes the supersaturation for *Is* and *Vs*. The current global concentration is calculated involving a time average between the current time and the last snapshot:

```
sprocess> LogFile [kmc extract supersaturation name=I]
1.00555
```

To obtain the supersaturation evolution with time, use the KMC Movie parameter as shown in the following example:

```
SetAtomistic
set kmcSupersat ""
pdbSet KMC MaxYum 30e-3
pdbSet KMC MaxZum 30e-3
pdbSet KMC Movie {lappend kmcSupersat $time [kmc extract \
    supersaturation name=I]}
pdbSet KMC automaticRampUp 1
line x loc=0.0    tag=xleft   spacing = 0.002
line x loc=1.5e-3 tag=xmed    spacing = 0.002
line x loc=350e-3 tag=xright  spacing = 0.002
region oxide    xlo=xleft xhi=xmed
region silicon  xlo=xmed xhi=xright

init
implant Silicon energy=40 dose=2e13 tilt=7
diffuse time=100000<s> temp=600
LogFile $kmcSupersat
```

This example produces the results:

```
10.0007 4.29101e+07
21.5462 2.51728e+07
46.4218 1.58636e+07
100.004 1.41889e+07
215.493 7.67109e+06
464.238 3.44625e+06
```

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### Extracting KMC-Related Information

```
1000.26 1.86513e+06
2156.46 477255
4645.69 322049
10002.8 113849
21551.6 132116
46419.1 110329
100006 81506.4
```

Figure 69 shows a comparison with experimental results.

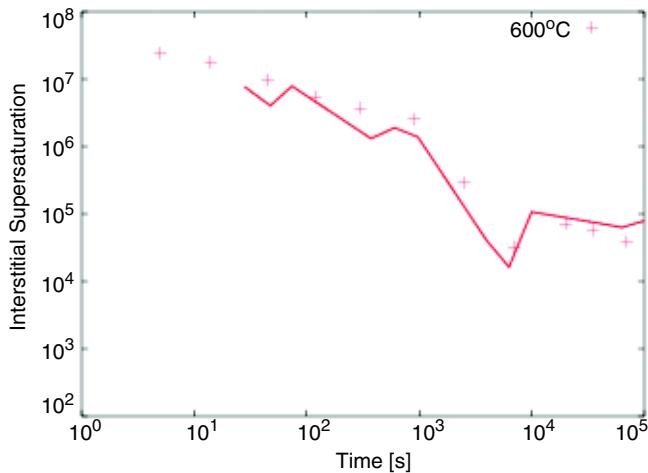


Figure 69 Supersaturation evolution with time, after a silicon implantation ( $2 \times 10^{13}$  dose, 40 keV energy) annealed  $1 \times 10^5$  s at 600°C. (Experimental points modified from [52] to use the same B diffusivity.) Points are experiments, lines are KMC.

### Extracting Raw Atomistic Information

The `defects` option allows access to the raw atomistic information of any simulation. The obtained information must match the arguments `name` and `defectname` when they are specified:

```
kmc extract defects name=<c> defectname=<c> [countparticles] [countdefects]
[materialname=<c>] [acinterface]
```

where:

- `name` can be a particle (B, A<sub>i</sub>) or a cluster (I<sub>n</sub>V<sub>m</sub>, B<sub>n</sub>I<sub>m</sub>).
- `defectname` can be ThreeOneOne, Interface, Loop, and so on.

When there are no restrictions, all defects are accessed. For example, for the following added defects:

```
kmc add queue name=BI2 coordx=2<nm> coordy=2<nm> coordz=3<nm>
kmc add queue name=I2 coordx=3<nm> coordy=2e-3 coordz=4e-3
```

```
kmc add queue name=I3 coordx=4<nm> coordy=3<nm> coordz=1<nm>
kmc add
```

The obtained defects are:

```
sprocess> kmc extract defects
0.00201273      0.00238963 0.00298179   I ImpurityCluster 0
0.00196125      0.00204962 0.00249501   I ImpurityCluster 0
0.00177392      0.00225923 0.00247647   B ImpurityCluster 0
0.00320253      0.00162722 0.00466375   I AmorphousPocket 1
0.00222551      0.00139856 0.004411     I AmorphousPocket 1
0.0044946       0.00317389 0.00130069   I AmorphousPocket 2
0.00441116      0.00353071 0.000842549  I AmorphousPocket 2
0.00403856      0.00351353 0.00084327   I AmorphousPocket 2
sprocess> kmc extract defects name=I
0.00201273      0.00238963 0.00298179   I ImpurityCluster 0
0.00196125      0.00204962 0.00249501   I ImpurityCluster 0
0.00320253      0.00162722 0.00466375   I AmorphousPocket 1
0.00222551      0.00139856 0.004411     I AmorphousPocket 1
0.0044946       0.00317389 0.00130069   I AmorphousPocket 2
0.00441116      0.00353071 0.000842549  I AmorphousPocket 2
0.00403856      0.00351353 0.00084327   I AmorphousPocket 2
sprocess> kmc extract defects name=I defectname=ImpurityCluster
0.00201273      0.00238963 0.00298179   I ImpurityCluster 0
0.00196125      0.00204962 0.00249501   I ImpurityCluster 0
sprocess> kmc extract defects name=BI2
0.00201273      0.00238963 0.00298179   I ImpurityCluster 0
0.00196125      0.00204962 0.00249501   I ImpurityCluster 0
0.00177392      0.00225923 0.00247647   B ImpurityCluster 0
```

The six columns present in the output are:

- X-coordinate of the defect
- Y-coordinate of the defect
- Z-coordinate of the defect
- Particle name
- Defect name.
- Number of defect. Particles with the same number belong to the same defect.

**NOTE** The `kmc extract defects` command can produce large outputs.

When there are amorphous defects in the simulation, the result may not be the expected. Amorphous defects do not store damage, but only its concentration (see [Amorphous Defects on page 451](#)). Consequently, amorphous defects will not report any interstitial or vacancy inside them. Impurities are stored and displayed. Nevertheless, if the indirect diffusion model is used in amorphous silicon, the dangling bonds, the floating bonds, and the mobile and

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### Extracting KMC-Related Information

immobile impurities will be obtained as I, V, Bi and B (for boron) (see [Indirect Diffusion Model on page 453](#)).

The argument `materialname` restricts the output to the material specified instead of the entire simulation.

The options `countparticles` and `countdefects` do not display atomistic information, but they count the number of particles and defects, respectively, for the given conditions. This example shows how to count the particles and defects listed in the previous example:

```
sprocess> kmc extract defects countparticles
8
sprocess> kmc extract defects countdefects
3
sprocess> kmc extract defects name=I countparticles
7
sprocess> kmc extract defects name=I defectname=AmorphousPocket countdefects
2
```

The option `acinterface` displays the lattice atoms belonging to the amorphous–crystalline interface. All the lattice atoms can be obtained using `acinterface detailed`, which generates output only when the LKMC model is used for recrystallization (see [LKMC: Fully Atomistic Modeling of Solid Phase Epitaxial Regrowth on page 458](#)).

## Extracting Concentration per Surface Unit

The `dose` option extracts the concentration per surface unit ( $\text{cm}^{-2}$ ) for the entire simulation cell, and it can be used to look at the evolution of the species with time:

```
kmc extract dose name=<c> defectname=<c> [countdefects] [materialname=<c>]
```

where:

- `name` can be any particle ( $I$ ,  $\text{AsV}$ ,  $B_i^-$ ) or any defect ( $I_n$ ,  $V_n$ ,  $I_nV_m$ ,  $B_nI_m$ ). It also can be a ‘total’ name – the name of an impurity followed by `Total` (`AsTotal`, `BTOTAL`) – and applies to all circumstances where the specified impurity is present, that is, in clusters, substitutional, pairs, and so on.
- `defectname` can be `ImpurityCluster`, `ThreeOneOne`, and so on. It can be specified only when `name` is a particle, and it restricts the particles to the specified type.

The arguments `name` and `defectname` restrict the species to compute the dose.

A list of defect types is obtained with `kmc defecttypes`.

This command counts the number of particles (such as `kmc extract defects` with the same restrictions and the `countparticles` option) and it divides this number by the surface

area. The argument materialname restricts the output to the material specified instead of the entire simulation. For interfaces, instead of specifying a material name, specify a particle name such as AsInterface, BIInterface.

As an example, the following command file implants silicon into silicon and extracts the dissolution of {311} defects during annealing:

```

set silicon_depth 350e-3
set size 50e-3
set SiO2gate 1.5e-3
SetAtomistic
set sol ""
pdbSet KMC Movie {lappend sol $time [kmc extract dose name=I \
    defectname=ThreeOneOne]}
pdbSet KMC MaxZum $size
pdbSet KMC MaxYum $size
pdbSet KMC GasUm $SiO2gate
pdbSet KMC automaticRampUp true
line x loc=0.0          tag=xtop      spacing = 0.002
line x loc=$silicon_depth tag=xbottom spacing = 0.002
region silicon xlo=xtop xhi=xbottom

init
deposit oxide fill coord=[expr -$SiO2gate]
implant silicon energy=40 dose=5e13 tilt=7
diffuse time=3100 temp=670
LogFile $sol

```

This example produces the results:

```

46.4176 2.88e+12
100.01 9.56e+12
215.464 1.104e+13
464.175 1.596e+13
1000 2.172e+13
2154.45 3.144e+13
4641.63 3.736e+13
10000 3.044e+13
21544.5 1.388e+13
46417.4 9.6e+11
100233 0

```

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### Extracting KMC-Related Information

Figure 70 shows the comparison with experimental data [8].

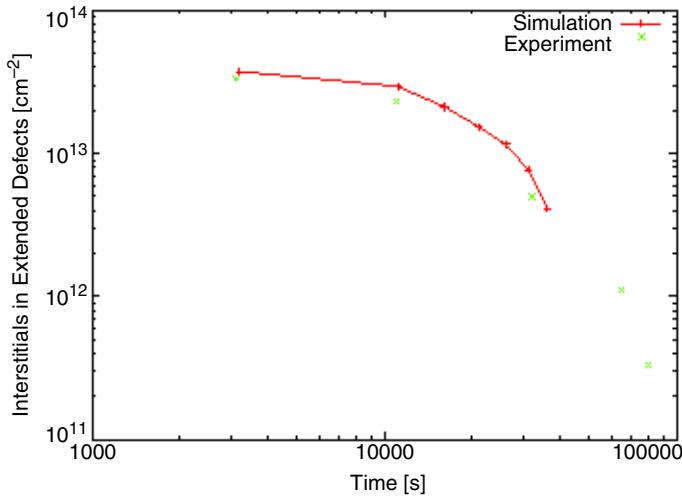


Figure 70 Dissolution of {311} extended defects at 670°C after a silicon into silicon implantation of 40 keV,  $5 \times 10^{13} \text{ cm}^{-2}$

## Extracting List of Materials

To extract a list of materials currently in the simulation, use:

```
kmc extract materials [coordx=<n>] [coordy=<n>] [coordz=<n>] [detailed]
```

For example:

```
sprocess> kmc extract materials  
Silicon Oxide Gas
```

The option detailed produces a list of coordinates and materials. This list contains the same number of dimensions as the simulation (except if you use coordx, coordy, or coordz). For example, in a 1D simulation:

```
sprocess> kmc extract materials detailed  
-0.002 Gas  
-0.000625 Oxide  
0.00075 Oxide  
0.002125 Oxide  
0.0035 Oxide  
0.004875 Oxide  
0.00625 Oxide  
0.007625 Oxide  
0.009 Oxide  
0.010375 Silicon  
0.01175 Silicon  
0.013125 Silicon
```

```
0.0145 Silicon
0.015875 Silicon
0.01725 Silicon
```

The arguments `coordx`, `coordy`, and `coordz` affect the output of `detailed` by changing its dimensionality. They work exactly the same as in `kmc extract profile` (see [Extracting Concentrations on page 547](#)).

## Extracting Amorphous–Crystalline Interfaces

To extract a list of amorphous–crystalline interfaces found in the simulation given a 1D cutline, use:

```
kmc extract acinterface [coordx=<n>] [coordy=<n>] [coordz=<n>]
```

No options are needed in one dimension. In two dimensions, you must specify `coordx` or `coordy`. In three dimensions, you must specify two of `coordx`, `coordy`, and `coordz`. For example, in one dimension:

```
sprocess> kmc extract acinterface
Silicon Amorphous/Crystalline 0.0165
```

When the KMC model for SPER is detected, the option `acinterface` displays all the places where the amorphous–crystalline field crosses the threshold specified in KMC `ACInterfaceAt`. A value of 1 means perfectly amorphous and 0 means perfectly crystalline. The default value is 0.9. The output also displays the materials at both sides of the interface, showing first the material with a smaller coordinate value. In this case, the interface is at 0.0165 μm, and the transition is from Amorphous to Crystalline as the x-coordinate increases. When the LKMC model is used for SPER, the parameter `ACInterfaceAt` is ignored, and a more precise interface is extracted directly from the LKMC atomistic information.

---

## Common Dopant and Point-Defect Names

Several options of the `kmc` command use the `name=<c>` argument. [Table 64 on page 558](#) lists several of these names and the commands where they are applicable. Since dopants can be defined as needed, the names depend on the simulation parameters. In particular, they contain names defined when using Advanced Calibration.

A list of the names can be obtained using `kmc particletypes` (see [Particle Types on page 401](#)). Clusters also are included in the list. Since the number of different clusters is large, only a partial cluster list is included as an example (see [Table 65 on page 561](#)).

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### Extracting KMC-Related Information

The kmc commands considered in these reference tables, and the symbols used to represent them, are:

- kmc add queue (Add)
- kmc deatomize (Dea)
- kmc extract defects (Def)
- kmc extract dose (Dos)
- kmc extract histogram (His)
- kmc extract profile (Pro)
- kmc extract supersaturation (Sup)
- kmc present (Pre)

The defects used in the descriptions are:

- Point defects, self-silicon point defects like interstitials and vacancies.
- Extended defects, agglomeration of self-silicon point defects.
- Clusters, agglomeration of impurities or dopants, with or without point defects.
- Substitutional dopants or impurities.
- Paired dopants or impurities, paired with point defects.
- Amorphous pockets, agglomeration of point defects (also sometimes called *damage*).
- Defects attached to interfaces.

Table 64 Names used in Sentaurus Process KMC

Name	Description	Used in
I	Neutral interstitial in point defects, clusters, and extended defects	Sup, His, Add, Pro, Dos, Def, Dea, Pre
IMM	$I^-$ , point defect	Add, Pro, Dos, Def, Dea, Pre
IM	$I^0$ , point defect	Add, Pro, Dos, Def, Dea, Pre
IP	$I^+$ , point defect	Add, Pro, Dos, Def, Dea, Pre
IPP	$I^{++}$ , point defect	Add, Pro, Dos, Def, Dea, Pre
ITotal	Total interstitial concentration; similar to I + IMM + IM + IP + IPP	Dea, Pre, Pro, Dos
V	Neutral vacancy in point defects, clusters, and extended defects	Sup, His, Add, Pro, Dos, Def, Dea, Pre
VMM	$V^{--}$ , point defect	Add, Pro, Dos, Def, Dea, Pre
VMM	$V^-$ , point defect	Add, Pro, Dos, Def, Dea, Pre
VM	$V^0$ , point defect	Add, Pro, Dos, Def, Dea, Pre

Table 64 Names used in Sentaurus Process KMC

Name	Description	Used in
VP	$V^+$ , point defect	Add, Pro, Dos, Def, Dea, Pre
VPP	$V^{++}$ , point defect	Add, Pro, Dos, Def, Dea, Pre
VPPP	$V^{+++}$ , point defect	Add, Pro, Dos, Def, Dea, Pre
VTotal	Total vacancy concentration; similar to $V + VMMM + VMM + VM + VP + VPP + VPPP$	Dea, Pre, Pro, Dos
B	Boron, substitutional, at interfaces or in clusters	Add, Pro, Dos, Def, Dea, Pre
BV	Neutral-paired defect, boron vacancy	Add, Pro, Dos, Def, Dea, Pre, His
BVM	$BV^-$ , paired defect	Add, Pro, Dos, Def, Dea, Pre
BVP	$BV^+$ , paired defect	Add, Pro, Dos, Def, Dea, Pre
Bi	Neutral-paired defect, boron interstitial	Add, Pro, Dos, Def, Dea, Pre, His
BiM	$Bi^-$ , paired defect	Add, Pro, Dos, Def, Dea, Pre
BiP	$Bi^+$ , paired defect	Add, Pro, Dos, Def, Dea, Pre
BTOTAL	Total boron concentration; similar to $B + BV + BVM + BVP + Bi + BiM + BiP$	Dea, Pre, Pro, Dos
BInterface	Boron at interfaces	Add, Pro, Dos, Def, Dea, Pre
As	Arsenic, substitutional at interfaces or in clusters	Add, Pro, Dos, Def, Dea, Pre
AsV	Neutral-paired defect of arsenic and a vacancy	Add, Pro, Dos, Def, Dea, Pre, His
AsVM	$AsV^-$ , paired defect	Add, Pro, Dos, Def, Dea, Pre
AsVP	$AsV^+$ , paired defect	Add, Pro, Dos, Def, Dea, Pre
Asi	Neutral-paired defect of arsenic and an interstitial	Add, Pro, Dos, Def, Dea, Pre, His
AsiM	$Asi^-$ , paired defect	Add, Pro, Dos, Def, Dea, Pre
AsiP	$Asi^+$ , paired defect	Add, Pro, Dos, Def, Dea, Pre
AsTOTAL	Total arsenic; similar to $As + AsV + AsVM + AsVP + Asi + AsiM + AsiP$	Dea, Pre, Pro, Dos
AsINTERFACE	Arsenic attached at interfaces	Add, Pro, Dos, Def, Dea, Pre
C	Carbon, substitutional, at interfaces or in clusters	Add, Pro, Dos, Def, Dea, Pre
CV	Neutral-paired defect of carbon and a vacancy	Add, Pro, Dos, Def, Dea, Pre, His
Ci	Neutral-paired defect of carbon and an interstitial	Add, Pro, Dos, Def, Dea, Pre, His
CINTERFACE	Carbon attached at interfaces	Add, Pro, Dos, Def, Dea, Pre
CTOTAL	Total carbon; similar to $C + CV + Ci$	Dea, Pre, Pro, Dos

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Table 64 Names used in Sentaurus Process KMC

Name	Description	Used in
F	Fluorine, substitutional at interfaces or in clusters	Add, Pro, Dos, Def, Dea, Pre
FI	Neutral-paired defect of fluorine with an interstitial	Add, Pro, Dos, Def, Dea, Pre, His
FV	Neutral-paired defect of fluorine with a vacancy	Add, Pro, Dos, Def, Dea, Pre, His
FTotal	Total fluorine; similar to F + FI + FV	Dea, Pre, Pro, Dos
FInterface	Fluorine attached at interfaces	Add, Pro, Dos, Def, Dea, Pre
In	Indium, substitutional, at interfaces or in clusters	Add, Pro, Dos, Def, Dea, Pre
InV	Neutral-paired defect of indium and a vacancy	Add, Pro, Dos, Def, Dea, Pre, His
InVM	InV <sup>-</sup> , paired defect	Add, Pro, Dos, Def, Dea, Pre
InVP	InV <sup>+</sup> , paired defect	Add, Pro, Dos, Def, Dea, Pre
Ini	Neutral-paired defect of indium and an interstitial	Add, Pro, Dos, Def, Dea, Pre, His
IniM	Ini <sup>-</sup> , paired defect	Add, Pro, Dos, Def, Dea, Pre
IniP	Ini <sup>+</sup> , paired defect	Add, Pro, Dos, Def, Dea, Pre
InTotal	Total indium; similar to In +InV + InVM + InVP + Ini + IniM + IniP	Dea, Pre, Pro, Dos
InInterface	Indium attached at interfaces	Add, Pro, Dos, Def, Dea, Pre
P	Phosphorus, substitutional, at interfaces or in clusters	Add, Pro, Dos, Def, Dea, Pre
PV	Neutral-paired defect of phosphorus and a vacancy	Add, Pro, Dos, Def, Dea, Pre, His
PVM	PV <sup>-</sup> , paired defect	Add, Pro, Dos, Def, Dea, Pre
PVP	PV <sup>+</sup> , paired defect	Add, Pro, Dos, Def, Dea, Pre
Pi	Neutral-paired defect of phosphorus and an interstitial	Add, Pro, Dos, Def, Dea, Pre, His
PiM	Pi <sup>-</sup> , paired defect	Add, Pro, Dos, Def, Dea, Pre
PiP	Pi <sup>+</sup> , paired defect	Add, Pro, Dos, Def, Dea, Pre
PTotal	Total phosphorus; similar to P + PV + PVM + PVP + Pi + PiM + PiP	Dea, Pre, Pro, Dos
PInterface	Phosphorus attached at interfaces	Add, Pro, Dos, Def, Dea, Pre
Sb	Antimony, substitutional, at interfaces or in clusters	Add, Pro, Dos, Def, Dea, Pre
SbV	Neutral-paired defect of antimony and a vacancy	Add, Pro, Dos, Def, Dea, Pre, His
SbVM	SbV <sup>-</sup> , paired defect	Add, Pro, Dos, Def, Dea, Pre

Table 64 Names used in Sentaurus Process KMC

Name	Description	Used in
SbVP	SbV <sup>+</sup> , paired defect	Add, Pro, Dos, Def, Dea, Pre
Sbi	Neutral-paired defect of antimony and an interstitial	Add, Pro, Dos, Def, Dea, Pre, His
SbiP	Sbi <sup>+</sup> , paired defect	Add, Pro, Dos, Def, Dea, Pre
SbTotal	Total antimony; similar to Sb + SbV + SbVM + SbVP + Sbi + SbiP	Dea, Pre, Pro, Dos
SbInterface	Antimony at interfaces	Add, Pro, Dos, Def, Dea, Pre
N	Nitrogen, substitutional, at interfaces or in clusters	Add, Pro, Dos, Def, Dea, Pre
NTotal	Total nitrogen, same as N	Dea, Pre, Pro, Dos
NInterface	Nitrogen at interfaces	Add, Pro, Dos, Def, Dea, Pre
Nn	N <sub>2</sub> , substitutional, at interfaces or in clusters	Add, Pro, Dos, Def, Dea, Pre
NnV	Moving N <sub>2</sub> V particle	Add, Pro, Dos, Def, Dea, Pre, His
NnTotal	Similar to Nn + NnV	Dea, Pre, Pro, Dos
NnInterface	N <sub>2</sub> stored at the interface	Add, Pro, Dos, Def, Dea, Pre
H	Hydrogen, substitutional, at interfaces or in clusters	Add, Pro, Dos, Def, Dea, Pre
HTotal	Total hydrogen, only H	Dea, Pre, Pro, Dos
HInterface	Hydrogen at interfaces	Add, Pro, Dos, Def, Dea, Pre
Ge	Germanium (stored as a field, not as a particle)	Add, Pro, Dos, Def, Dea, Pre

Table 65 Some cluster names used in Sentaurus Process KMC

Name	Description	Used in
IV	Interstitial–vacancy amorphous pocket.	His, Add, Pro, Dos, Def, Dea, Pre
I <sub>x</sub> V <sub>y</sub>	Amorphous pocket. Any other I <sub>x</sub> V <sub>y</sub> with x and y integers is also valid.	Add, Pro, Dos, Def, Dea, Pre
I <sub>8</sub>	Extended defect formed by eight interstitials. Any other I <sub>x</sub> , where x is an integer, is also valid.	Add, Pro, Dos, Def, Dea, Pre
V <sub>x</sub>	Extended defect formed by four vacancies. Any other V <sub>x</sub> , where x is an integer, is also valid.	Add, Pro, Dos, Def, Dea, Pre
B <sub>2</sub> I <sub>3</sub>	Boron–interstitial cluster. Other integers are also valid.	Add, Pro, Dos, Def, Dea, Pre
As <sub>4</sub> V	Arsenic–vacancy cluster. Other integers are also valid.	Add, Pro, Dos, Def, Dea, Pre

Table 65 Some cluster names used in Sentaurus Process KMC

Name	Description	Used in
B2IC3	Dopant cluster. Any combination of dopants with (or without) interstitials or vacancies is valid.	Add, Pro, Dos, Def, Dea, Pre
P2As2I	Another example for dopant cluster	Add, Prod, Dos, Def, Dea, Pre

---

## Advanced Calibration for Sentaurus Process KMC

**NOTE** The use of Advanced Calibration is strongly recommended.

The default parameters used in Sentaurus Process KMC are inherited from previous versions of Sentaurus Process KMC and may not be accurate for modern processing conditions. A more accurate calibration for Sentaurus Process KMC has been performed by the Advanced Calibration team and is available using the command:

```
AdvancedCalibration
```

This command includes the calibration of KMC models for point-defects and dopants in Si, SiGe, and Ge, as well as LKMC models for SPER and epitaxy of Si, SiGe and Ge.

This command must be written after `SetAtomistic` since it detects the presence of an atomistic simulation to load the Advanced Calibration parameters related to Sentaurus Process KMC:

```
SetAtomistic  
...  
AdvancedCalibration
```

In cases where Advanced Calibration for Sentaurus Process KMC must be loaded without calling `SetAtomistic` in advance, you must use the `KMC` flag as follows:

```
AdvancedCalibration KMC
```

In particular, this is the preferred mode to call Advanced Calibration for Sentaurus Process KMC in hybrid simulations, and the only way to do it when using the `kmc` option of the `diffuse` command.

**NOTE** For more information on the Advanced Calibration parameters and methodology, refer to the *Advanced Calibration for Process Simulation User Guide*.

---

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# Lattice Kinetic Monte Carlo: Epitaxial Deposition

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*This chapter describes the atomistic simulation approach to epitaxial deposition in Sentaurus Process.*

Epitaxial deposition methods described in [Epitaxy on page 267](#) are based on the conventional (continuum) simulation approach. The atomistic approach to epitaxial deposition described here is based partially on the kinetic Monte Carlo (KMC) diffusion simulator DADOS [\[1\]](#)[\[2\]](#)[\[3\]](#) and is available with the optional Sentaurus Process Kinetic Monte Carlo license.

---

## Overview of Epitaxial Deposition

Sentaurus Process Lattice Kinetic Monte Carlo (Sentaurus Process LKMC) is coupled to Sentaurus Process Kinetic Monte Carlo (Sentaurus Process KMC), and handles epitaxial deposition and solid phase epitaxial regrowth (SPER). This chapter focuses on epitaxial deposition using Sentaurus Process LKMC. For more information about SPER, see [LKMC: Fully Atomistic Modeling of Solid Phase Epitaxial Regrowth on page 458](#).

The basis setup for the fully atomistic mode or hybrid mode for Sentaurus Process LKMC is the same as described for Sentaurus Process KMC in [Operating Modes on page 374](#).

Using a method similar to continuum-style simulations, epitaxial deposition in Sentaurus Process LKMC is divided into a sequence of time steps, where each time step is composed of the following in this order:

1. A doped deposition step using either native LKMC or continuum Sentaurus Process
2. Update of continuum Sentaurus Process structure and a mechanics step
3. An atomistic KMC diffusion step

In addition to using continuum deposition (see [Epitaxy on page 267](#)), several native LKMC options are available to perform part 1 of each time step, which is described in the rest of this section.

To use one of the native LKMC models:

- In atomistic mode, you must specify: `pdbSet KMC Epitaxy True`
- In nonatomistic or hybrid mode, you must specify `1kmc` in the `diffuse` command.

## 6: Lattice Kinetic Monte Carlo: Epitaxial Deposition

### Planar Epitaxy Models

When used in nonatomic mode with `1kmc` specified in the `diffuse` command, doping and diffusion are controlled by the continuum solver. Sentaurus Process LKMC controls the deposition shape (see [Using LKMC for Deposition Shape on page 268](#)).

---

## Epitaxy Models

The following classes of epitaxy models are available:

- One class is based on planar considerations as described in [4] and includes the `Planes` and `Coordinations.Planes` models.
- One class is based on atomic bonding energies and includes the `Coordinations.Reactions` and `Coordinations` models.

The growth and reaction rates in the `Coordinations.Reactions` and `Coordinations` models are determined by the *coordination*, that is, the number and type of bonds between the depositing species and those in the deposition surface. In addition, the model `Coordinations.Reactions` considers reactions that occur during chemical vapor deposition (CVD). Examples of such reactions include decomposition of source gases, site blocking effects of a *carrier* gas such as H<sub>2</sub>, and desorption of source gas molecules. The `Coordinations` model does not consider reactions, but still includes the growth rate dependency on the composition and crystal orientation of the deposition surface.

The growth rate in the planar models `Coordinations.Planes` and `Planes` is based on the growth rate of important surface orientations. The difference between these two models is the increased configurability of the `Coordinations.Planes` model over the `Planes` model. The default growth rate for these models is the same.

To choose an epitaxy model, specify:

```
pdbSet LKMC Epitaxy.Model <model>
```

where `<model>` is `Coordinations`, `Coordinations.Reactions`, `Planes`, or `Coordinations.Planes`.

---

## Planar Epitaxy Models

The `Coordinations.Planes` model and the `Planes` model introduce a lattice for the depositing atoms based on the starting growth surface and assign a status to each lattice site (either empty or filled). Then, Sentaurus Process LKMC assigns a fill rate to all the empty sites. The growth rate of the empty sites is determined by the orientation of the neighboring filled (already deposited) sites, and only empty sites next to filled sites have a rate different from zero.

Both models use the same material parameters and the same species-independent LKMC atom creation and management algorithms. However, the `Coordinations.Planes` model uses flexible Tcl callback procedures to set the parameters of the model.

These models share many features with the SPER model (see [LKMC: Fully Atomistic Modeling of Solid Phase Epitaxial Regrowth on page 458](#)).

The growth rate for an empty site substrate–gas interface is:

$$v_{\text{Epi}} = K' \times v_{\text{SEG}}^{\text{LKMC}} \quad (841)$$

where  $v_{\text{SEG}}^{\text{LKMC}}$  is the frequency for selective epitaxial growth (SEG), very similar to the one written in [Eq. 732, p. 460](#):

$$v_{\text{SEG}}^{\text{LKMC}} = K_{\text{SEG}}^{\text{LKMC}}(\text{site}) \times \exp\left(-\frac{E_{\text{SEG}}^{\text{LKMC}} + \Delta E(\text{site})}{k_B T}\right) \quad (842)$$

$K_{\text{SEG}}^{\text{LKMC}}(\text{site})$  is a prefactor that accounts for the local microscopic growth for each configuration. This prefactor depends on the following variables:

- $n$  can be 100, 110, or 111 defined very similarly to K(1), K(2), and K(3) in [LKMC: Fully Atomistic Modeling of Solid Phase Epitaxial Regrowth on page 458](#).
- $m$  is used to distinguish between configurations with the same  $n$  but different second-neighbor coordination numbers.

In this model, also published in [4], 100 configurations only are split into three different ones: 100, 100.7, and 100.8 for 100 configurations with six or fewer, seven, and 8 or more second-neighbor coordination numbers.

$\Delta E(\text{site})$  is a correction energy applied to special sites. It is used to simulate the formation of {311} facets during SEG. As such, only one site is defined to have a non-null correction: the {311} local configuration.

This configuration is in two different situations:

- (a) is a (100) generic site that lacks half of its third neighbors.
- (b) is a (110) site where the second atom in the chain needed to define the place as 110 would have its first coordination number equal to 2.

Assigning a slower rate to configuration (a) prevents a {311} facet becoming a {111} facet. The slower rate for configuration (b) ensures that the local {311} configuration is not broken by a lateral (110) regrowth.

## 6: Lattice Kinetic Monte Carlo: Epitaxial Deposition

### Planar Epitaxy Models

$K'$  is an empirical factor and can be set in one of the following ways depending on whether `epi.thickness` is specified in the `diffuse` command:

- With `epi.thickness` specified, this factor fits the epitaxial deposition thickness to the specified thickness. Sentaurus Process LKMC computes this empirical factor automatically, trying to match the thickness specified in the processing conditions. In particular:

$$K' = K_{\text{thickness}} \times \frac{\text{thickness}}{v_{\text{SEG}}^{\text{LKMC}}(100) \times \text{time} \times K_{\text{nanolayer}}} \quad (843)$$

where:

- `thickness` is the specified thickness.
- `time` is the annealing time.
- $K_{\text{nanolayer}}$  is the thickness of a monolayer of recrystallized silicon. A monolayer is assumed to be half the lattice constant.
- $v_{\text{SEG}}^{\text{LKMC}}(100) = K(100) \times \exp\left(-\frac{E_{\text{SEG}}^{\text{LKMC}}}{k_B T}\right)$  is the frequency for recrystallization in a pure (100) substrate.
- $K_{\text{thickness}}$  is an empirical constant, available as `Epitaxy prefactor.thickness` in the Parameter Database (PDB), which relates the microscopic growth of a lattice atom in a (100) local neighborhood with the macroscopic growth of a (100) substrate.
- Without `epi.thickness` specified, it is assumed that the growth parameters have been calibrated to a particular process. If this is the case, the  $\langle 100 \rangle$  growth rate will depend on the temperature in addition to its usual dependency on the local microstructure. For convenient calibration, when `epi.thickness` is not specified, the overall empirical prefactor  $K'$  is set to the `prefactor.thickness` parameter.

**NOTE** Because `prefactor.thickness` has been roughly calibrated for Eq. 843, this quantity is probably too large for the mode where `epi.thickness` is *not* specified in the `diffuse` command. In such cases, the default deposition rate can be high. It is recommended to start with `prefactor.thickness` values less than 0.01 and to increase values until a reasonable growth rate is achieved.

This epitaxial deposition can create {111} facets and maintain the same (100):(110):(111) growth rate as SPER. Under regular selective epitaxial conditions, the shapes generated agree with experimental ones.

**NOTE** To avoid problems, the `KMC Movie` command is switched off during LKMC epitaxy. In addition, the `diffuse movie` command must not be used during LKMC epitaxial deposition.

## Parameters of the Planar Epitaxy Models

Parameters of these models are defined in the PDB under KMC Si Epitaxy.

Table 66 Parameters for the site prefactors for different site types

Parameter	Description
prefactor.SEG.100.8	For (100) sites with 8 or more second-neighbor coordination number.
prefactor.SEG.100.7	For (100) sites with 7 second-neighbor coordination number.
prefactor.SEG.100	For (100) sites with 6 or fewer second-neighbor coordination number.
prefactor.SEG.110	For (110) sites.
prefactor.SEG.111	For (111) sites.

In addition to the separate prefactors for SEG for different site types, there are separate energy barriers associated with different site types. The default value for all the anisotropic barriers is 0.0 (that is, isotropic energy barriers) with a nonzero overall activation energy given by `energy.SEG`. The one exception to isotropic default barriers is an energy *correction* for the {311} site type, which is given an extra barrier.

Table 67 Parameters for the SEG activation energies and thickness

Parameter	Description
<b>SEG activation energies</b>	
energy.SEG	Overall activation energy for SEG. This energy is added to all sites. The default is material dependent.
energy.SEG.311	Correction for {311} planar SEG. The default is material dependent.
energy.SEG.100.8	For (100) sites with 8 or more second-neighbor coordination numbers. Default: 0.0.
energy.SEG.100.7	For (100) sites with 7 second-neighbor coordination numbers. Default: 0.0.
energy.SEG.100	For (100) sites with 6 or fewer second-neighbor coordination numbers. Default: 0.0.
energy.SEG.110	For (110) sites. Default: 0.0.
energy.SEG.111	For (111) sites. Default: 0.0.
<b>Thickness</b>	
prefactor.thickness	Empirical factor to fit the thickness in epitaxial growth.

---

## Dopant-Dependent Growth Rate Factor

To add a dopant-dependent growth rate, specify the following PDB parameters:

```
pdbSetDouble <material> KMC Epitaxy <dopant> Growth.Rate.Factor.0 <n>
pdbSetDouble <material> KMC Epitaxy <dopant> Growth.Rate.Factor.E <n>
```

**NOTE** Both parameters can be positive or negative, and both default to 0.

The growth rate is modified by a factor DDGRF, where:

$$\text{DDGRF} = 1 + r_0 e^{\frac{-r_E}{kT}} \text{ <dopant mole fraction>} \quad (844)$$

where:

- The parameter  $r_E$  is given by Growth.Rate.Factor.E.
- The parameter  $r_0$  is given by Growth.Rate.Factor.0.

These parameters will be mole fraction–interpolated like the other growth parameters.

---

## Epitaxy Models Based on Atomic Bonding

The Coordinations and Coordinations.Reactions models have more capabilities than the planar epitaxy models. They both allow for multiple depositing species and have species-dependent growth rates that depend on the composition of the deposition surface in addition to its orientation. The Coordinations.Reactions model is the most complete, allowing for the simulation of chemical reactions during growth.

The following effects can be simulated using the Coordinations model:

- Mole fraction–dependent growth rate
- Dopant-dependent growth rate
- Mole fraction dependency on surface orientation, and dopant concentration
- Dopant concentration dependent on surface orientation and mole fraction
- Atomistic handling of dopants, and transfer directly to Sentaurus Process KMC for diffusion
- Twin-defect formation during epitaxy
- Segregation of species from the surface to the bulk

In addition to these effects, the `Coordinations.Reactions` model includes:

- Carrier gas effects such as reduced growth rate due to site blocking
- Temperature-activated decomposition of source gas to material atoms
- Temperature-activated desorption of molecules such as those from carrier gas, source gas, or surface reaction products
- Etching
- Mimicking dangling bonds by a shared site occupancy model

## Running the `Coordinations` and `Coordinations.Reactions` Models

These physically based models depend on process conditions such as gas flows and temperature for input instead of relying on users to specify the final results such as thickness, mole fraction, and doping levels. As such, these models are invoked differently from other epitaxy models requiring the use of the `gas_flow` command to set the flow rate of the source, dopant, and carrier gases as well as temperature and time.

As previously mentioned, the `Coordinations` and `Coordinations.Reactions` models require the specification of epitaxial gas conditions. This is accomplished by specifying ambients in the `diffuse`, `temp_ramp`, or `gas_flow` commands. Several ambients have been predefined for this purpose (see [Table 68](#)).

**Table 68** Predefined ambients for use with `Coordinations` and `Coordinations.Reactions` models

Ambient name	Formula	LKMC atom name	Number of atoms	Molecular mass [amu]
Arsine	AsH <sub>3</sub>	Arsenic	1	77.9
Borane	BH <sub>3</sub>	Boron	1	13.8
Diborane	B <sub>2</sub> H <sub>6</sub>	Boron	2	27.7
Dichlorosilane	SiH <sub>2</sub> Cl <sub>2</sub>	Silicon	1	101.0
Disilane	Si <sub>2</sub> H <sub>6</sub>	Silicon	2	62.2
Germane	GeH <sub>4</sub>	Germanium	1	76.6
Phosphine	PH <sub>3</sub>	Phosphorus	1	34.0
Silane	SiH <sub>4</sub>	Silicon	1	32.1
H <sub>2</sub>	H <sub>2</sub>	HStar	2	6.1
HGas	H <sub>2</sub>	HStar	2	6.1

## 6: Lattice Kinetic Monte Carlo: Epitaxial Deposition

### Epitaxy Models Based on Atomic Bonding

Table 68 Predefined ambients for use with Coordinations and Coordinations.Reactions models

Ambient name	Formula	LKMC atom name	Number of atoms	Molecular mass [amu]
HCl	HCl	HClStar	1	36.4
HClGas	HCl	HClStar	1	36.4

For example, to specify boron-doped SiGe epitaxy, use the following commands:

```
gas_flow name= SiGe_Bdope flowSilane= 0.75 flowGermane= 0.25 \
flowBorane= 0.0002 pressure= 1.0<torr> epi
diffuse time= 2<s> temperature=375 gas.flow= SiGe_Bdope
```

Because deposition and doping rates depend on the growth rate parameters, the mole fraction in this example will not necessarily be 0.25, and the doping concentration will not necessarily be  $2.0 \times 10^{-4} / \text{lattice density}$ . Only if the parameters are the same for Si, Ge, and B would the example be true.

**NOTE** As is the case with oxidation, you can set the gas flow specification (that is, `flow<Ambient>`) not only in the `gas_flow` command, but also as a shorthand directly in the `temp_ramp` or `diffuse` command.

You can also define your own ambient if one of the predefined ambients is not sufficient. The `lkmc.atom.name`, `lkmc.mass`, and `lkmc.num.atoms` arguments of the `ambient` command are specific to the Coordinations model.

The list of available LKMC atoms is taken from the PDB parameter `Periodic.Table`, which is at the highest level in the PDB. The `lkmc.mass` argument of the `ambient` command specifies the molecular weight of the gas delivering the atom named in `lkmc.atom.name`. The `lkmc.num.atoms` argument is used for molecules containing more than one LKMC atom, for example, diborane ( $\text{B}_2\text{H}_6$ ). The default for `lkmc.num.atoms` is 1.

The following ambient commands correspond to the definition of germane ( $\text{GeH}_4$ ), disilane ( $\text{Si}_2\text{H}_6$ ), and borane ( $\text{BH}_3$ ) from [Table 68 on page 573](#):

```
ambient name= Germane Epi add lkmc.mass= 76.6<amu> lkmc.atom.name= Germanium
ambient name= Disilane Epi add lkmc.mass= 62.2<amu> lkmc.atom.name= Silicon \
lkmc.num.atoms= 2
ambient name= Borane Epi add lkmc.mass= 13.8<amu> lkmc.atom.name= Boron
```

The unit `<amu>` is atomic mass unit or gram/mole.

**NOTE** The parameter Epi (or LTE or user-defined ‘Epi’ ambient) must be specified in the same location that the LKMC atom ambients are specified (either the `gas_flow` or `diffuse` command). The material names, both deposited and seed, are determined by this parameter along with reactions defined by the `reaction` command.

## Growth Rate of the Coordinations Model

The growth rate of species  $i$  for site configuration  $c$  in the Coordinations model is given as:

$$R_i(c) = J_i f_i^0(c) \exp\left(\frac{-E_i(c)}{kT}\right) \quad (845)$$

where  $J_i$  is the arrival rate of species  $i$  and the rest of the expression:

$$f_i^0(c) \exp\left(\frac{-E_i(c)}{kT}\right) \quad (846)$$

can be considered to express the fraction of gas molecules arriving at the surface that deposit on or adsorb to a site of coordination  $c$ . Note that  $E_i$  would also represent the energy to break up the gas molecule and diffuse to the growth site minus the binding energy of the molecule to the surface.

The molecular arrival rate is a well-known expression in the kinetic theory of gases:

$$\begin{aligned} J_i &= \frac{n_i \langle v_i \rangle}{4} \\ &= \frac{P_i}{RT} \sqrt{\frac{8kT}{\pi m_i}} \\ &= 3.93 \times 10^{10} \frac{P_i}{\sqrt{m_i T}} \text{ site}^{-1} \text{ s}^{-1} \end{aligned} \quad (847)$$

where:

- $P_i$  is the partial pressure of the gas delivering species  $i$  in atmosphere.
- $m_i$  is the mass of the gas molecule delivering species  $i$  in atomic mass unit (g/mol). This expression assumes a site density of  $6.78 \times 10^{14} \text{ cm}^{-2}$ , which is the approximate density of deposition sites on the  $<100>$  surface of silicon.
- $f_i^0(c)$  set by:

```
pdbSet <epi_material> LKMC <Ambient/EpiAtom> prefactor.SEG.ads <n>
```

where:

- `<epi_material>` is the name of the depositing material.

## 6: Lattice Kinetic Monte Carlo: Epitaxial Deposition

### Epitaxy Models Based on Atomic Bonding

- <Ambient/EpiAtom> is Ambient for the Coordinations model and EpiAtom for the Coordinations.Reactions model.
- $E_i(c)$  can be considered a coordination-dependent formation energy and is given (for nonpassivating surface species) by:

$$E_i(c) = E_{0i} - \sum_j (nn_j Enn_{ij} + nnn_j Ennn_{ij} + n3_j^{rd} E3_{ij}^{rd}) \quad (848)$$

where:

- $nn_j$  is the number of nearest neighbors of species type  $j$ .
- $nnn_j$  is the number of second-nearest neighbors of species type  $j$ .
- $n3_j^{rd}$  is the number of third-nearest neighbors of species type  $j$ .
- $Enn_{ij}$  is the binding energy between epi species  $i$  and the nearest-neighbor surface species type  $j$  and is set with:

```
pdbSet <epi_material> LKMC <ambient/epi_species> <surface_species> \
energy.SEG.bNnn <n>
```

- $Ennn_{ij}$  is the binding energy between epi species type  $i$  and the second-nearest neighbor surface species type  $j$  and is set with:

```
pdbSet <epi_material> LKMC <ambient/epi_species> <surface_species> \
energy.SEG.bNnnn <n>
```

- $E3_{ij}^{rd}$  is the binding energy between epi species type  $i$  and the third-nearest neighbor surface species type  $j$  and is set with:

```
pdbSet <epi_material> LKMC <ambient/epi_species> <surface_species> \
energy.SEG.bN3rd <n>
```

- $E_{0i}$  is the coordination and surface species-independent energy barrier for epi species  $i$  to reach a growth site and is set with:

```
pdbSet <epi_material> LKMC <ambient/epi_species> energy.SEG.ads <n>
```

---

## Coordinations.Reactions Model

This model was developed to model chemical reactions during CVD epitaxy to improve growth rate accuracy, especially temperature and gas flow rate effects, which cannot be modeled with simpler models where the growing species deposit at a rate nearly independent of other gases present during growth.

The Coordinations.Reactions model is set up as a series of chemical reactions, including adsorption, surface reactions including decomposition of source gases into their growing

component atoms, desorption, and etching. The only reactions considered occur at the surface, so that the product of any gas reactions away from the surface is taken as input for the model.

A default set of reactions is available in the `SPROCESS.models` file (see [Environment Variables on page 13](#) for information on how to find this file). The commands used to set up the model are described here to assist in understanding the model and to allow the model to be extended to include new effects.

The reactions of the model are specified using the `reaction` command. The adsorption reactions require specification of an LKMC ambient created with the `ambient` command. The species involved in the reactions can come from different sources: ambients, atoms defined with the PDB parameter `Periodic.Table`, which is at the highest level in the PDB, and newly created species specifically for the `Coordinations.Reactions` model using the parameter `LKMC.Species`.

To add a new species, use:

```
pdbSet LKMC Species <species_name> <surface_type>,<site_specification>
```

where:

- `<species_name>` is the name of the new LKMC species.
- `<surface_type>` can be either `Grow` or `Passivate` to specify whether atoms can be deposited on this species or not, respectively.
- `<site_specification>` can be A, B, or AB to indicate the site validity for lattices with different lattice types. In Version N-2017.09, this setting has no effect, but it will be enabled in a future release.

To create a new ambient for LKMC, specify:

```
ambient lkmc name=<c> lkmc.mass=<n> [<amu>]
```

The `lkmc.mass` argument specifies the mass of the ambient molecule. The unit `<amu>` is available to indicate atomic mass unit.

To specify the following types of reaction, use these commands:

- Adsorption:

```
reaction lkmc ambients= {<ambient1>=<n> <ambient2>=<n> ...} \
products= {<product1>=<n> <product2>=<n> ...}
```

- Surface reaction:

```
reaction lkmc reactants= {<reactant1>=<n> <reactant2>=<n> ...} \
products= {<product1>=<n> <product2>=<n> ...}
```

- Desorption:

```
reaction lkmc reactants= {<reactant1>=<n> <reactant2>=<n> ...}
```

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- Etching:

```
reaction lkmc ambients= {<ambient1>=<n> <ambient2>=<n> ...} \
    reactants= {<reactant1>=<n> <reactant2>=<n> ...}
```

Here,  $<n>$  indicates the stoichiometry of the species in the reaction.

## Reaction Rates in the Coordinations.Reactions Model

Reaction rates in the Coordinations.Reactions model are based on the same formation energies as the Coordinations model given in [Eq. 848, p. 576](#) except the Coordinations.Reactions model introduces the concept of passivating species. Passivating species such as H tend to relax dangling surface bonds, and so the model assumes a barrier for incorporating growing or doping species next to or on top of a passivating species. The convention for passivating species is to use the suffix Star, so H is referred to as HStar.

The coordination-dependent energies for passivating species are set independently of the depositing species type (although the coordination-independent energy,  $E_{0i}$ , is the same). Therefore, [Eq. 848](#) becomes:

$$E_i^*(c) = E_{0i} - \sum_j (nn_j Enn_j + nnn_j Ennn_j + n3_j^{rd} E3_j^{rd}) \quad (849)$$

where:

- $nn_j$  is the number of nearest neighbors of species type  $j$ .
- $nnn_j$  is the number of second-nearest neighbors of species type  $j$ .
- $n3_j^{rd}$  is the number of third-nearest neighbors of species type  $j$ .
- $Enn_j$  is the binding energy between any epi species and the nearest-neighbor passivating surface species type  $j$  and is set with:

```
pdbSet <epi_material> LKMC <surface_species> energy.SEG.bNnn <n>
```

- $Ennn_j$  is the binding energy between any epi species and the second-nearest neighbor passivating surface species type  $j$  and is set with:

```
pdbSet <epi_material> LKMC <surface_species> energy.SEG.bNnnn <n>
```

- $E3_j^{rd}$  is the binding energy between any epi species and the third-nearest neighbor surface species type  $j$  and is set with:

```
pdbSet <epi_material> LKMC <surface_species> energy.SEG.bN3rd <n>
```

- $E_{0i}$  is the same as in [Eq. 848](#).

The prefactor for reaction rates is set with the prefactor argument of the reaction command. There is also an additional energy barrier available with the energy argument of the reaction command. To set the prefactor or energy, you must redefine the equation. This

can be performed by copying the equation from the `SPROCESS.models` file to your command file, and adding the specification of the prefactor or energy.

The reaction rate for surface reactions is given by  $R_{\text{surf}} = r_0 e^{\frac{-E}{k_B T}}$  where:

$$E = E_0 + f_r \sum_r E_r(c) + f_p \sum_p E_p(c) \quad (850)$$

and:

- $r_0$  is given by the `prefactor` argument of the `reaction` command (default 1.0).
- $E_0$  is given by the `energy` argument of the `reaction` command (default 0.0).
- $f_r$  is given by the `reactants.efactor` argument of the `reaction` command (default -1.0).
- $f_p$  is given by the `products.efactor` argument of the `reaction` command (default +1.0).
- $E_r(c)$  and  $E_p(c)$  are given by [Eq. 848](#).

For adsorption reactions, the rate is given by  $R_{\text{ads}} = r_0 J_i e^{\frac{-E}{k_B T}}$ , where  $E$  is given by [Eq. 850](#) with no reactants,  $J_i$  is given by [Eq. 847](#), and  $r_0$  is given by the `prefactor` argument of the `reaction` command.

For desorption reactions, the rate is  $R_{\text{des}} = r_0 e^{\frac{-E}{k_B T}}$ , where  $E$  is given by [Eq. 850](#) with no products, and  $r_0$  is given by the `prefactor` argument of the `reaction` command.

For etching reactions, the rate is  $R_{\text{etch}} = r_0 J_i e^{\frac{-E}{k_B T}}$ , where  $E$  is given by [Eq. 850](#) with no products,  $J_i$  is given by [Eq. 847](#), and  $r_0$  is given by the `prefactor` argument of the `reaction` command.

## Parameters of the Epitaxy Models Based on Atomic Bonding

[Table 69](#) and [Table 70 on page 580](#) summarize the parameters for both the `Coordinations` and `Coordinations.Reactions` models. The parameters in [Table 69](#) are at the following level for both the `Coordinations` model and the nonpassivating surface species of the `Coordinations.Reactions` model:

```
<epi_material> LKMC <epi_species> <surface_species>
```

For the passivating species in the `Coordinations.Reactions` model, the parameters are at the level:

```
<epi_material> LKMC <surface_species>
```

Table 69 Parameters for the Coordinations and Coordinations.Reactions models

Parameter	Description
energy.SEG.bNnn	Nearest-neighbor binding energy (usually, a negative number) in eV.
energy.SEG.bNnnn	Second-nearest neighbor binding energy (usually, a negative number) in eV.
energy.SEG.bN3rd	Third-nearest neighbor binding energy (usually, a negative number) in eV.

The parameters in [Table 70](#) are at the <epi\_material> LKMC <epi\_species> level for the Coordinations.Reactions model and at the <epi\_material> LKMC <ambient> level for the Coordinations model.

Table 70 Surface species-independent parameters for the Coordinations and Coordinations.Reactions models

Parameter	Description
prefactor.SEG.ads	Adsorption prefactor.
energy.SEG.ads	Binding energy of the ambient or epi atom to any surface atom. When using surface species-independent binding, you must set the species-dependent binding energies (in <a href="#">Table 69</a> ) to 0 and vice versa.

## Boundary Conditions

In Version M-2016.12 or earlier, the Coordinations and Coordinations.Reactions models were available only with periodic boundary conditions, irrespective of the boundary conditions applied to the KMC domain.

In Version N-2017.09, reflective boundary conditions have been enabled for these models and, by default, LKMC epitaxy will follow the boundary conditions available for the KMC domain, which can be set by the following commands:

```
pdbSet KMC PeriodicBC.Y <true | false>
pdbSet KMC PeriodicBC.Z <true | false>
```

**NOTE** You can use the following command to force periodic boundary conditions for the LKMC epitaxy models, but it is *not* recommended to force periodic boundary conditions in this way:

```
pdbSetBoolean LKMC Force.PeriodicBC true
```

---

## Controlling Point-Defect Injections at Interfaces and Their Diffusion

Fast-moving point defects might result in LKMC simulations that appear very slow or unresponsive. For example, if an interstitial is injected from the interface during LKMC, it will continue to diffuse until there is a reason to slow down or it is annihilated by recombining with a vacancy. Such diffusion events can be a few orders of magnitude faster than LKMC events such as adsorption or etching and, therefore, the simulation appears frozen. To control such injections, you can switch off injection of these point defects from the interface during LKMC or reduce the diffusivity of interstitials and vacancies by scaling down the diffusivity.

By default, injection at interfaces depends on the interface model. You can switch off injection of point defects from the interface by setting the following parameter (default is `true`):

```
pdbSet <interface_mat> LKMC KMC.Injection false
```

A more convenient way to switch on or off these interface injections for LKMC is to call the `SetInterfaceInjectionLKMC` procedure, set to either `true` or `false`. Calling this procedure ensures that, when reading the parameters, these injection settings are applied to all available interfaces.

To scale down the diffusivity of interstitials and vacancies during LKMC, set the following diffusivity scaling parameters:

```
pdbSet <mat> LKMC Interstitial Dm.Scaling <0-1>
pdbSet <mat> LKMC Interstitial Em.Scaling <0-1>
pdbSet <mat> LKMC Vacancy Dm.Scaling <0-1>
pdbSet <mat> LKMC Vacancy Em.Scaling <0-1>
```

The range of values allowed for these scaling parameters is between 0 and 1, with a default value of 1.

---

## Modifying and Extending the Epitaxy Models

To make the models as flexible and configurable as possible, Tcl callback procedures allow you to specify a large number of parameters using scripting. This enables the specification of prefactors and energy functions based on the number of bonds for any combination of depositing species and surface species. In addition, scripting allows you to handle exceptional species combinations for fine-tuning or calibration.

The `Coordination` model, the `Coordination.Reactions` model, and to a lesser extent the `Coordination.Planes` model can be modified in the command file by redefining

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### Modifying and Extending the Epitaxy Models

internally specified Tcl procedures. These procedures are found in the `LKMC.tcl` file, which is located in the `$STROOT/tcad/$STRELEASE/lib/sprocess/TclLib/tcl` directory.

The relevant callback procedures are:

- `LKMCEpiEnergy` sets the growth rate energy barrier that depends on the depositing species (either dopant, material, or alloy atom) and also can be made a function of the number of neighbors of each species on the surface.
- `LKMCEpiPrefactor` sets the species-dependent growth rate prefactor. The prefactor depends on the incoming species and can also depend on the species-independent neighbors on the surface. To reduce the complexity of calibration, you should set the prefactors to be independent of the surface configuration (and to depend only on the depositing species).
- `LKMCEpiFactor0` sets an overall growth rate prefactor.
- `LKMCEpiFactorE` sets an overall growth rate barrier.

The calling parameter for all these procedures is a Tcl list that creates a Tcl array containing parameter names as the array index and parameter values as the indexed array value. For example, to override the internal `LKMCEpiEnergy` callback procedure, use:

```
proc LKMCEpiEnergy { args } {
    array set argArr $args
    set Nnn $argArr(Nnn)
    set Nnnn $argArr(Nnnn)
    set N3rd $argArr(N3rd)
    set GasNeighborNN $argArr(GasNeighborNN)
    set MoleFraction $argArr(MoleFraction)
    set EpiMat $argArr(EpiMat)
    set Base0 $argArr(Base0)
    set Base1 $argArr(Base1)
    set BaseMat $argArr(BaseMat)
    set energy <compute energy here using $Nnn, $Nnnn, $N3rd, and so on>
    return $energy
}
```

Table 71 Calling parameters for the `LKMCEpiEnergy` and `LKMCEpiPrefactor` callback procedures of the `Coordinations.Planes` model

Parameter name	Description
<code>Base0</code> , <code>Base1</code>	This is the material corresponding to mole fractions of 0 and 1, respectively. For example, if <code>EpiMat</code> is <code>SiliconGermanium</code> , then <code>Base0==Silicon</code> when <code>MoleFraction==0</code> .
<code>EpiMat</code>	Name of the material to be deposited.
<code>GasNeighborNN</code>	Maximum number of nearest neighbors of all neighboring gas sites.

**Table 71** Calling parameters for the LKMCEpiEnergy and LKMCEpiPrefactor callback procedures of the Coordinations.Planes model

Parameter name	Description
MoleFraction	Value can be 0 or 1. For alloys, the procedure is called twice, once for mole fraction 0 and once for mole fraction 1.
N3rd	Number of third nearest neighbors.
Nnn	Number of nearest neighbors.
Nnnn	Number of next-nearest neighbors.

The epitaxy factor is defined by:

$$F_{\text{epi}} = \frac{x_{\text{epi}}}{t_{\text{epi}} l_{\text{epi}}} f_0 \exp\left(-\frac{f_E}{kT}\right) \quad (851)$$

where:

- $f_0$  is the result of the Tcl procedure `LKMCEpiFactor0`.
- $f_E$  is the result of the Tcl procedure `LKMCEpiFactorE`.
- $x_{\text{epi}}$  is the epitaxy thickness specified in the `temp_ramp` or `diffuse` command.
- $t_{\text{epi}}$  is the epitaxy time specified in the `temp_ramp` or `diffuse` command.
- $l_{\text{epi}}$  is the thickness of one monolayer of epitaxial material.

The `LKMCEpiFactor0` and `LKMCEpiFactorE` callback procedures are provided for backward compatibility. They are used to obtain a scaling factor applied to all deposition rates both for when `epi.thickness` is specified and for when it is not specified.

**Table 72** Calling parameters for the LKMCEpiFactor0 and LKMCEpiFactorE callback procedures of the Coordinations.Planes model

Parameter name	Description
Base0, Base1	This is the material corresponding to mole fractions of 0 and 1, respectively. For example, if <code>EpiMat</code> is <code>SiliconGermanium</code> , then <code>Base0==Silicon</code> when <code>MoleFraction==0</code> .
EpiMat	Name of the material to be deposited.
MoleFraction	Value can be 0 or 1. For alloys, the procedure is called twice, once for mole fraction 0 and once for mole fraction 1.
thicknessSpecified	Value can be 1 or 0, depending on whether <code>epi.thickness</code> was used in the specification of deposition conditions.

The calling parameter `EpiAtom` is one of the atoms being deposited, and the parameter `SurfaceAtom` is one of the atoms already deposited or initialized from the seed material. In

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### Modifying and Extending the Epitaxy Models

addition, `SurfaceAtom` can be the special atom type `Any`. When `Any` is passed in, it allows the energy to be set independently of the species of the `SurfaceAtom`.

Because growth energies are summed (species dependent and species independent), it is possible to obtain backward compatibility for the previous species-independent `Planes` model (by setting all species-dependent parameters to zero). Conversely, you can specify a pure bond-counting species-dependent model by setting the species-independent parameters (that is, `SurfaceAtom==Any` to zero). In addition, a combination is possible where you start with the previous species-independent parameters and add small species-dependent corrections to it.

Because the `LKMCEpiEnergy` and `LKMCEpiPrefactor` procedures implement the parameters used in the `Planes` model, this corrective scheme can be implemented easily by renaming the internal procedures and defining your own, for example:

```
rename LKMCEpiPrefactor internalLKMCEpiPrefactor
proc LKMCEpiPrefactor { args } {
    array set argArr $args

    if {$argArr(Nnn) > 2} {
        set val [expr 2.0 * [eval internalLKMCEpiPrefactor $args]]
        #LogFile IL0 "Nnn: $argArr(Nnn) - $val"
        return $val
    }
    return [eval internalLKMCEpiPrefactor $args]
}
```

This procedure returns twice the default value if the number of nearest neighbors is greater than 2. Otherwise, it returns the default value. You can uncomment the `LogFile IL0...` line to see the actual values returned.

---

## Orientation-Dependent Prefactors in the Coordinations.Reactions Model

There are callback procedures to apply a multiplication factor to rates of specific reactions depending on the local neighbor configuration. This provides flexibility for calibration purposes. The following callback procedures, available in the `LKMC.tcl` file, enable such multiplication factors:

- `LKMCApplyOrientFactor_CR` takes a reaction name as its argument and returns whether to apply such factors for this reaction. This helps to limit the effect on performance due to additional parameter settings and lookup, by limiting such multiplication factors to specific reactions. By default, it returns false for all reactions.
- `LKMCEpiOrientFactor_CR` can be set for specific reactions and defines the multiplication factors depending on neighbour configuration.

- `LKMCReactionOrientFactor_CR` internally calls `LKMCEpiOrientFactor_CR` and sets those multiplication factors for specific reactions. For example, to apply such factors to a reaction named `Silane_ads`, specify:

```
proc LKMCReactionOrientFactor_CR { args } {
    if { $args(ReactionName) == "Silane_ads" } {
        return [expr 0.1*[LKMCEpiOrientFactor_CR $args]
    } else {
        return [LKMCEpiOrientFactor_CR $args]
    }
}
```

The reaction rate is modified depending on the local neighbor configuration by  $\text{ModifiedRate} = \text{factor} \times \text{Rate}$ .

The default definition of `LKMCEpiOrientFactor_CR` uses the parameters in [Table 73](#), and the procedure definition is similar to `LKMCEpiPrefactor_CP` in terms of defining certain neighbor configurations for a particular orientation.

**Table 73** Default factor parameters called in `LKMCEpiOrientFactor_CR`

Parameters	Description
Factor.SEG.100	Multiplication factor for <100> orientation. Default: 1.
Factor.SEG.110	Multiplication factor for <110> orientation. Default: 1.
Factor.SEG.111	Multiplication factor for <111> orientation. Default: 1.
Factor.SEG.311	Multiplication factor for <311> orientation. Default: 1.

**NOTE** The orientation definitions in `LKMCEpiPrefactor_CP` are based on neighbor configurations for adsorption on a perfect surface, and the same is defined for `LKMCEpiOrientFactor_CR`. For a reaction other than adsorption (for example, etching), you must define the correct neighbor configuration according to the reaction, to apply such factors correctly. For example, during adsorption, a growth site on a clean <111> surface has one nearest neighbor but, during etching, an etching site on a clean <111> surface can have one or three nearest neighbors.

You can define your own `LKMCEpiOrientFactor_CR` procedure for specific reactions and set specific factors depending on the local neighbor configuration.

The `LKMCEpiOrientFactor_CR` and `LKMCReactionOrientFactor_CR` procedures take the arguments in [Table 74 on page 586](#).

## 6: Lattice Kinetic Monte Carlo: Epitaxial Deposition

### Modifying and Extending the Epitaxy Models

Table 74 Parameters for the LKMCReactionOrientFactor\_CR and LKMCEpiOrientFactor\_CR callback procedures

Parameter	Description
GasNeighborNN	Maximum number of nearest neighbors of all neighboring gas sites.
Nnn	Number of nearest neighbors.
Nnnn	Number of second-nearest neighbors.
N3rd	Number of third-nearest neighbors.
ReactionName	Name of the reaction for which the procedure is being modified.

---

## SiGe and Mole Fraction–Dependent Growth

You can simulate homo-epitaxial growth of SiGe and Ge. By default, SiGe will be deposited on exposed SiGe regions or Ge will be deposited on Ge regions when the Epi option is specified in the diffuse command. However, you cannot deposit two different materials simultaneously. If such a condition is encountered, for example, when there are two or more exposed regions of silicon, SiGe, or germanium, and Epi is specified in the diffuse command, an error message is generated and Sentaurus Process LKMC stops.

The growth of SiGe and pure Ge uses the same model and parameters as the model for Si epitaxy as described in [Parameters of the Planar Epitaxy Models on page 571](#). Parameters for SiliconGermanium are by default interpolated from their value in the *base* materials, which in this case are Silicon and Germanium where the relative interpolation weight is based solely on the mole fraction specification in the diffuse command.

**NOTE** Because the Ge parameters have not been calibrated accurately, caution must be used when depositing both SiGe (due to its implicit reliance on Ge parameters) and Ge itself.

You can specify the mole fraction for SiliconGermanium epitaxy using the command MoleFractionFields (see [MoleFractionFields on page 1089](#)). To specify a graded doping from 0.1 to 0.5 mole fraction, the following can be added to the diffuse command:

```
diffuse ... time=<n> temperature=<n> Epi epi.thickness=<n> \
    epi.doping= "[MoleFractionFields SiliconGermanium 0.1]" \
    epi.doping.final= "[MoleFractionFields SiliconGermanium 0.5]"
```

In this example, the MoleFractionFields command will generate a specification for the Silicon and Germanium fields in SiliconGermanium.

You can also perform hetero-epitaxy using the ambient and reaction commands similar to continuum epitaxy. For example, to grow Germanium on Silicon, the following set of commands can be used:

```
# Create a new ambient so as not to interfere with default Epi ambient  
ambient name= GeEpi epi add  
  
# Next, create the new temporary material used during epi itself  
mater name=GeEpiOnSilicon add new.like= Germanium kmc.shortname= GeEpi  
  
# Ensure the new temporary material is active in KMC/LKMC  
pdbSet KMC Materials GeEpiOnSilicon true  
  
# Finally, specify the new reaction to grow on Silicon/Gas interface  
# The mat.final is the name of the material after diffusion  
# The name of the reaction is not important  
reaction name= GeOnSiliconReaction mat.l=Silicon mat.r=Gas \  
mat.new= GeEpiOnSilicon mat.final= Germanium ambient.name= GeEpi
```

During such growth, Ge is deposited on a Si lattice. Therefore, when transferring the mole fraction and alloy concentration, it can result in the overestimation of alloy concentration and mole fractions. To avoid overestimations or underestimations, you can apply a correction due to lattice density differences. Such a correction ensures that the mole fraction and alloy atoms are transferred according to [Eq. 316, p. 244](#). To switch on such a correction, set the following parameter:

```
pdbSet LKMC Lattice.Density.Correction true
```

---

## Visibility

By default, all empty sites are candidates for epitaxial growth. However, some gas sites can be cut off from the gas flow if material grows over a void leaving a trapped bubble of gas. After the gas has reacted with the surface of the bubble, no further deposition should occur.

To capture this effect, you must switch on visibility, using:

```
pdbSet LKMC Use.Visibility true
```

Visibility is available for the Coordinations and Coordinations.Reactions models.

## 6: Lattice Kinetic Monte Carlo: Epitaxial Deposition

### Modifying and Extending the Epitaxy Models

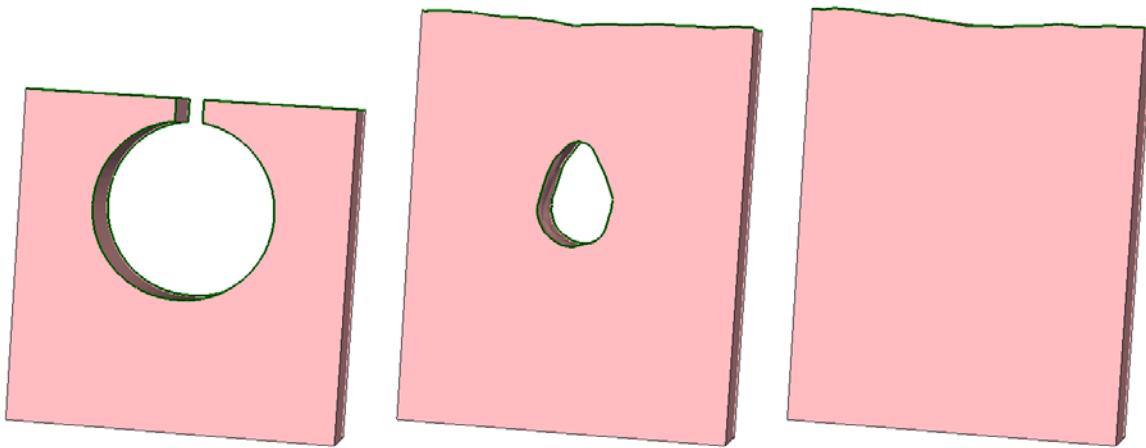


Figure 71 Simple example showing the effect of visibility: (*left*) the starting structure is a cavity with a small opening; (*middle*) during deposition with visibility switched on, growth occurs everywhere until the hole is filled, leaving a bubble; and (*right*) with visibility switched off, growth continues until no gas sites remain

---

## Twin-Defect Formation

In addition to the previously mentioned parameters, you can enable twin-defect formation along the  $<111>$  direction using the following setting:

```
pdbSet LKMC Epitaxy.Twin.Model <option>
```

The available options are `None` (default) and `OneOneOne`. When you use the `OneOneOne` option, the probability of twinning occurring in the  $<111>$  direction is taken as 0.5, that is, the lattice will grow in either perfect orientation or the twinned orientation.

You can also control the cleaning of lattice atoms at the end of diffusion steps by the following setting:

```
pdbSet LKMC Epitaxy.Cleanup <true | false>
```

To prevent the cleaning of lattice atoms, thereby enabling the visualization of lattice atoms in different twin orientations, specify:

```
pdbSet LKMC Epitaxy.Cleanup false
```

## Surface Segregation

The epitaxy models based on atomic bonding also allow species in the bulk to segregate to the surface. Surface segregation is modeled as a two-site exchange reaction for both the Coordinations and Coordinations.Reactions models, that is, the species participating in the segregation reaction exchange their sites.

The rate of segregation is given by:

$$\text{prefactor} \times \exp\left(-\frac{E_a}{kT}\right) \quad (852)$$

where:

- prefactor is the prefactor of segregation defined in the reaction command, multiplied by prefactor.segregation defined in [Table 75 on page 590](#).
- $E_a$  is defined in [Figure 72](#) and in the subsequent description of this quantity.

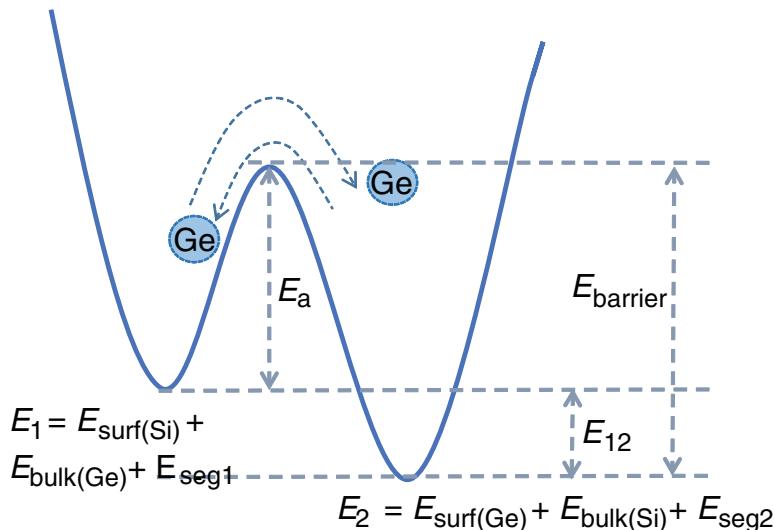


Figure 72 Energy diagram for surface segregation reaction in SiGe

[Figure 72](#) shows an example of an energy diagram for surface segregation in SiGe, where Ge is the bulk species before segregation and becomes the surface species after segregation, sending Si atoms into the bulk.

## 6: Lattice Kinetic Monte Carlo: Epitaxial Deposition

### Modifying and Extending the Epitaxy Models

The quantities shown in [Figure 72 on page 589](#) are:

- $E_1$  and  $E_2$  are the total formation energies in the states *before* the species are exchanged and *after* the species are exchanged, respectively.
- $E_{\text{bulk}}$  is the energy of the respective species in the bulk, which is calculated by  $\sum nn_j \cdot Enn_j$  where  $Enn$  is the nearest-neighbor binding energy as given in [Table 69 on page 580](#).
- $E_{\text{surf}}$  is the energy of the respective species in the surface, which is calculated similarly to  $E_{\text{bulk}}$ .
- $E_{\text{seg}1}$  and  $E_{\text{seg}2}$  are the segregation energies for Si and Ge *before* the species are exchanged and *after* the species are exchanged, respectively. These can be set as described in [Table 75](#).
- $E_{12}$  is the energy difference between the two states of the system, before and after segregation:

$$E_{12} = E_1 - E_2 \quad (853)$$

- $E_{\text{barrier}}$  is an additional reaction barrier.
- $E_a$  is the activation energy for the surface segregation reaction given by  $E_{\text{barrier}} - E_{12}$ .

A reaction definition is required to enable such species segregation. You can define a segregation reaction as:

```
reaction lkmc name=<c> segregation= <list> prefactor=<n> energy=<n>
```

The `segregation` argument specifies the two species participating in the segregation reaction, thereby exchanging places near the surface during growth. The `prefactor` argument is a multiplication factor to the segregation prefactor of the segregating species (see [Table 75](#)), and the `energy` argument is the energy barrier (see  $E_{\text{barrier}}$  in [Figure 72](#)) provided by users.

Table 75 Parameters for surface segregation of species

Parameter	Description
<code>prefactor.segregation</code>	Species-specific prefactor parameter for surface segregation.
<code>energy.segregation</code>	Species-specific segregation energy parameter for surface segregation.

The parameters for surface segregation can be set as:

```
pdbSet <mat> LKMC <bulk_atom> prefactor.segregation <n>
pdbSet <mat> LKMC <bulk_atom> <surface_atom> energy.segregation <n>
```

---

## Secondary Reactions: Allowing Products Leaving the Surface to Initiate New Reactions

The `Coordinations.Reactions` model enables capturing the influence of products leaving the reaction surface on the ambient fluxes using a simple model. The ambient flux in this case is modified as:

$$J_{\text{total}} = J_{\text{in}} + J_{\text{des}} \quad (854)$$

where:

- $J_{\text{in}}$  is the incoming ambient arrival rate as given by [Eq. 847, p. 575](#).
- $J_{\text{des}}$  is the desorption flux and is calculated by:

$$J_{\text{des}} = \text{factor} \times \frac{N_{\text{des}}}{\Delta t} \times \frac{1}{\text{Area}} \quad (855)$$

where:

- $N_{\text{des}}$  is the number of products leaving the surface influencing the desorption flux, over a time period given by  $\Delta t$ .
- *factor* is a user-defined factor of the overall desorption flux, which becomes part of the incoming flux.
- *Area* is the area over which influence of the desorption flux will be considered.

The effect of desorption fluxes on the ambient arrival rate is switched off by default and is switched on by the following setting:

```
pdbSet LKMC Epitaxy.Desorption.Flux true
```

In addition, reaction definitions as described in [Coordinations.Reactions Model on page 576](#) should be modified to include the products affecting ambients with the `ambient.products` argument of the `reaction` command. For example, a modified desorption reaction can be:

```
reaction name=<reaction_name> lkmc \
    reactants= {<reactant1>=<n1> reactant2=<n2>} \
    ambient.products= {<ambient1>=<n1> ...} prefactor=<pref> energy=<ener>
```

This reaction definition helps determine which ambient arrival rates will be affected by the products of this reaction.

**NOTE** For efficient updates, the ambient leaving as a reaction product should be part of the incoming gas flow. It is recommended to add such an ambient to the incoming gas flow, even with a very small partial pressure, to see the effect of the desorbed ambient.

## 6: Lattice Kinetic Monte Carlo: Epitaxial Deposition

### Modifying and Extending the Epitaxy Models

The desorbed ambient concentration is updated at a specified number of events and can be set by:

```
pdbSet LKMC Epitaxy.Desorption.Flux.Update <n>
```

The default value of this parameter is 50000. This parameter helps calculate the time difference  $\Delta t$  between subsequent updates. The area over which the influence of the desorption flux to be considered is defined (in  $\text{cm}^2$ ) by:

```
pdbSet LKMC Epitaxy.Desorption.Area <n>
```

By default, the desorption flux is calculated over the area of the entire simulation domain. The factor of the desorption flux calculation can be defined by:

```
pdbSet LKMC Epitaxy.Desorption.Flux.Factor <ambient_name> <n>
```

The default value of this factor is 0.

---

## Mimicking Dangling Bonds Using Shared Occupancy

When reactions produce passivating species, in reality, this species consumes one dangling bond. In LKMC, this species consumes one lattice site and, therefore, all the dangling bonds associated with the nearest neighbors to that lattice site. This situation is illustrated in Figure 73.

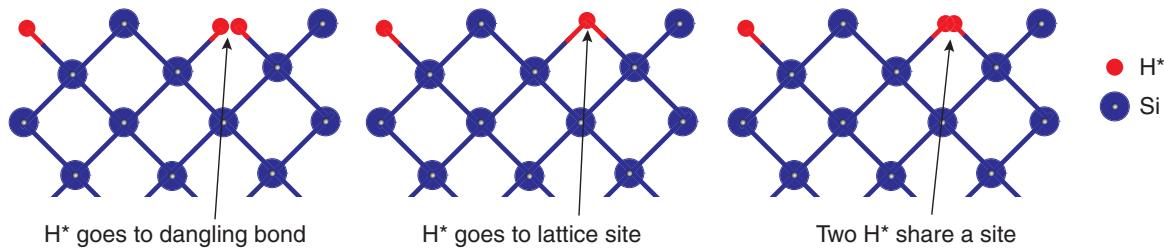


Figure 73 Illustration of how the shared occupancy model mimics dangling bonds and is a more physically correct approach than a model without shared occupancy: (left) the physical situation when  $\text{H}^*$  occupies a dangling bond; (middle) in the Coordinations.Reactions model without shared occupancy,  $\text{H}^*$  consumes both dangling bonds; and (right) shared occupancy allows two  $\text{H}^*$  to share the same lattice site, mimicking two dangling bonds

You can use the shared occupancy model to simulate a near-physical representation of dangling bonds using the Coordinations.Reactions model, which allows site sharing by more than one passivating species. The occupancy factor of a shared site is equal to the number of bonds to bulk species it creates, if it were occupied by a crystal atom (for example, Si, Ge, or dopants). In other words, the occupancy factor is equal to the number of dangling bonds it consumes.

To switch on the shared occupancy model, set the following parameter:

```
pdbSet LKMC Dangling.Bond.Model true
```

Sharing sites is allowed between passivating species and can be specified by the following parameter, for example:

```
pdbSet LKMC Shared.Occupancy { HStar,HStar,HStar true }
```

This example allows a site to be shared by a maximum of three H\* species. If a bulk species is present in the shared occupancy definition, it is ignored. For example, the following definition would be ignored:

```
pdbSet LKMC Shared.Occupancy { Silicon,HStar,HStar true }
```

A maximum of three species is allowed in such a definition, since certain surfaces can have three dangling bonds (for example, a (111) surface).

In such a situation with shared occupancy, counting the neighbors to the calculated formation energies without taking into account the effect of occupied dangling bonds might result in nonphysical rates. The following counting methods are available with this model:

- The default method is Count.All in which all neighbors are counted as is. Multiple species sharing a site are counted as individual neighbors. Using parameters calibrated without shared occupancy might result in an underestimation or overestimation of formation energies in such a case.
- The more detailed Count.DB method allows you to apply a penalty for the presence of dangling bonds in the neighbors.

You can specify the counting method by setting the following parameter:

```
pdbSet LKMC Dangling.Bond.Counting.Scheme <Count.All | Count.DB>
```

In the case of Count.DB, the penalty for occupied dangling bonds present in the nearest neighbor, second-nearest neighbor, and third-nearest neighbor can be set with the parameters in [Table 76 on page 594](#).

These parameters modify the coordination-dependent formation energy in [Eq. 849](#) as follows:

$$E_i^*(c) = E_{0i} - \left( \sum_j (nn_j E_{nnj} + nnn_j E_{nnnj} + n3_j^{rd} E_{3_j^{rd}}) - \sum_k (nn_k^{DB} E_{DB}^{DB} nn_k^{DB} + nnn_{kj}^{DB} E_{DB}^{DB} nnn_k^{DB} + n^{DB} 3_k^{rd} E_{DB}^{DB} 3_k^{rd}) \right) \quad (856)$$

## 6: Lattice Kinetic Monte Carlo: Epitaxial Deposition

### Modifying and Extending the Epitaxy Models

where:

- $nn_k^{\text{DB}}$ ,  $nnn_k^{\text{DB}}$ , and  $n_k^{\text{DB}}3_k^{\text{rd}}$  are the number of the nearest, second-nearest, and third-nearest neighbour dangling bonds, respectively.
- $E^{\text{DB}}nn_k^{\text{DB}}$ ,  $E^{\text{DB}}nnn_k^{\text{DB}}$ , and  $E^{\text{DB}}3_k^{\text{rd}}$  are penalties for occupied dangling bonds in the nearest, second-nearest, and third-nearest neighbors, respectively, as given in [Table 76](#).

The parameters in [Table 76](#) are at the following level for the nonpassivating surface species occupied by `epi_species` dangling bonds in their neighbors:

```
<epi_material> LKMC <epi_species> <surface_species>
```

**Table 76 Energies that provide the penalties for the presence of occupied dangling bonds in nearest, second-nearest, and third-nearest neighbors**

Parameter	Description
<code>energy.DB.bNnn</code>	Penalty parameter for presence of occupied dangling bonds in nearest neighbors.
<code>energy.DB.bNnnn</code>	Penalty parameters for presence of occupied dangling bonds in second-nearest neighbors.
<code>energy.DB.bN3rd</code>	Penalty parameters for presence of occupied dangling bonds in third-nearest neighbors.

For the passivating species in the `Coordinations.Reactions` model, the parameters are at the following level:

```
<epi_material> LKMC <surface_species>
```

---

## Nonselective Epitaxial Deposition of Polysilicon on Oxide

Experimentally, some polysilicon growth on exposed oxide or nitride material surfaces has been observed during epitaxy. It is possible to model such phenomena using the `Coordinations` and `Coordinations.Reactions` models.

These models mimic such events by a controlled nucleation of epitaxial islands on the oxide or nitride surface. They use the nearest-neighbor bonding strength of atoms at the interface with oxide or nitride and, therefore, they affect the rate of growth or etching of atoms close to such surfaces.

To enable nucleation of such islands on oxide or nitride material surfaces, you must specify a list of materials, for example:

```
pdbSet LKMC Nucleation.Materials {  
    Oxide true  
    Nitride false  
}
```

This list specifies the material on which you want to enable such nucleation. In this example, oxide is chosen for such nucleation.

A reaction definition for polysilicon growth on oxide must be defined as well, for example:

```
reaction name= PolyOnOxide ambient.name= Epi mat.l= Oxide mat.r= Gas \
mat.new= EpiOnOxide new.like= PolySilicon mat.final= PolySilicon \
mat.lattice.lkmc= Silicon
```

This reaction definition is similar to defining other epitaxy or low-temperature epitaxy (LTE) reactions, except that you specify `mat.lattice.lkmc` as well. Since there is no lattice information available for oxide material, this argument enables the use of the silicon lattice for oxide material. However, this results in the need for `AmorphousEpiOnOxide` material for the Sentaurus Process LKMC infrastructure. Therefore, it is recommended to switch off the use of this amorphous material using:

```
pdbSetString EpiOnOxide KMC Equivalent {}
pdbSetString AmorphousEpiOnOxide KMC Equivalent {}
```

You can also use the `mater` command to define `AmorphousEpiOnOxide` but, since it is not needed, it is better to switch off the equivalency as noted here.

For both the `Coordinations` and `Coordinations.Reactions` models, a nucleation reaction can be defined as a modified adsorption reaction by:

```
reaction name=<> lkmc ambients= {Silane= 1} products= {Silicon= 1} \
nucleation.material= {Oxide} energy=<> prefactor=<>
```

The `nucleation.material` argument identifies this definition as a nucleation reaction.

The argument `lkmc.nucleate` of the `temp_ramp` command or `diffuse` command triggers nucleation events. Therefore, in the case of multiple `temp_ramp` processes, nucleation events will not be triggered until the `temp_ramp` step containing `lkmc.nucleate` begins and any following `temp_ramp` steps will have nucleation switched on. This can be defined by either of the following commands:

```
temp_ramp ... lkmc.nucleate
diffuse ... lkmc.nucleate
```

In addition, the effect of bond strength on the oxide or nitride material surface can be enabled for other reactions in the `Coordinations.Reactions` model, without triggering nucleation. This can be switched on by the following setting:

```
pdbSet LKMC Non.Silicon.Bonding true
```

## 6: Lattice Kinetic Monte Carlo: Epitaxial Deposition

### Modifying and Extending the Epitaxy Models

Table 77 Parameters for setting bond strength and prefactor for nucleation reaction

Parameter	Description
prefactor.SEG	Prefactor parameter for nucleation
energy.SEG.bNnn	Energy or bond strength parameter for nucleation

The parameters in [Table 77](#) can be set as follows:

```
pdbSet Oxide LKMC prefactor.SEG <>
pdbSet Oxide LKMC <epiAtom> energy.SEG.bNnn <>
```

These parameters are similar to those determining binding energies and prefactors (see [Table 70 on page 580](#)).

## Calculating the Rate of the Nucleation Reaction

The rate of the nucleation reaction is given by:

$$R_{\text{Nucl}} = J_i f_n f_i^0(c) \exp\left(-\frac{E_i(c)}{kT}\right) \quad (857)$$

where, for the Coordinations model:

- $J_i$  is the ambient arrival rate.
- $f_n$  is the reaction prefactor given by the `reaction` command for the definition of the nucleation reaction.
- $f_i^0$  is the adsorption prefactor given by the `prefactor.SEG` parameter (see [Table 77](#)).
- $E_i(c)$  is the energy of the reaction given by:

$$E_i(c) = E_n - \sum_j (nn_j E_{nn_j} + nnn_j E_{nnn_j} + n3_j^{rd} E_{3_j^{rd}}) - \sum_k (nn_k E_{nn_k}) \quad (858)$$

where:

- $E_n$  is the energy given by the `reaction` command for the definition of the nucleation reaction.
- The first summation term is the total binding energy in the bulk material.
- The second summation term is the nearest-neighbor binding energy in the nucleation material, for example, oxide, calculated using `energy.SEG.bNnn` (see [Table 77](#)).

For the `Coordination.Reactions` model, in addition to all these terms for the nucleation rate calculation, rates of other reactions are adjusted by a modified  $E_i^*(c)$  from Eq. 849 as given by:

$$E_i^*(c) = E_{0i} - \sum_j (nn_j Enn_j + nnn_j Ennn_j + n3_j^{rd} E3_j^{rd}) - \sum_k (nn_k Enn_k) \quad (859)$$

Eq. 859 also applies if `Non.Silicon.Bonding` is set to true without triggering nucleation.

## Dopant Activation and Clustering During Epitaxy

You can control dopant activation and clustering during epitaxy using the parameters listed in Table 78.

Table 78 Parameters for controlling activation and clustering of dopants during epitaxy

Parameter	Description
<code>C0.Epi.Max.Active</code>	Prefactor for calculating the active dopant concentration during epitaxy. Default: 5e22
<code>E.Epi.Max.Active</code>	Energy for calculating the active dopant concentration during epitaxy. Default: 0.0
<code>Epi.Deposit.Active</code>	<code>DoubleArray</code> type. Determines the fraction of the active dopant that must be deposited either as a dopant (for example, boron as boron particles) or as dopant-defect pairs (for example, boron as Bi or BV). Default: <dopant> 1.0
<code>Epi.Deposit.Complex</code>	<code>DoubleArray</code> type. Determines the fraction of the active dopant that must be deposited into a particular size of cluster, and determines which cluster type to be deposited for the nonactive dopants. Multiple clusters and their fractions can be provided.

The `C0.Epi.Max.Active` and `E.Epi.Max.Active` parameters are used in an Arrhenius expression, given here, to calculate the dopant concentration that will remain active:

$$C0.Epi.Max.Active \times \exp\left(-\frac{E.Epi.Max.Active}{kT}\right) \quad (860)$$

## Updating the Finite-Element Structure During and After Epitaxy

The following operations occur at the end of LKMC epitaxial deposition:

- Sentaurus Process LKMC smooths the generated atomistic interface and reinserts it into the continuum simulator.
- The algorithm used to mesh the atomistic shape uses the `KMC Simplify.Geometry` parameter. A larger value provides faster insertion, but with a loss of surface details.

Before discussing boundary updating, it is worth noting that the inclusion of doping is possible during LKMC epitaxy and non-LKMC epitaxy. If a doping profile is specified, the included doping will be linear with time, *not* with thickness. You can also control the activation and clustering of dopant atoms. See [Table 78 on page 597](#) for a list of relevant parameters.

Several settings affect the quality and integrity of the boundary, which in turn can affect the mesh quality and robustness of the mesh generation. If a problem is encountered, try the following suggestions in the given order. You should continue to later suggestions only if necessary:

- To improve the boundary after insertion and before meshing, the boundary repair algorithm is called by default (see [Boundary Repair Algorithm on page 823](#)). In rare cases, this algorithm can use excessive memory or lead to an excessive simulation time. To switch off the algorithm, use:

```
pdbSet LKMC Boundary.Repair false
```

- If meshing fails after the structure is inserted, in some cases, adjusting the `mgoals` argument `repair.angle` can help. During repair, angles in the boundary smaller than this argument are targeted for removal. It can be increased, although a value of 5 is the largest recommended value, as follows:

```
mgoals repair.angle=5
```

- In atomistic mode, updating the partial differential equation (PDE) structure is a low priority. The only cases when it is mandatory are as follows:
  - When saving a TDR file
  - When mechanics updates are needed by Sentaurus Process KMC
  - When there are structural changes due to etching or deposition

Switching off automatic remeshing of the PDE structure could save time, while still allowing the same type of cleanup steps previously described to improve the boundary so that, when a mesh is needed, quality and stability are maintained.

**NOTE** Be aware that when saving a TDR file using either the `struct` command or the `kmc extract` command, with mesh update switched off, only the KMC grid is saved in the TDR file.

Files created when automatic remeshing of the PDE structure is switched off cannot be used for restarting.

The following parameter setting switches off mesh update after epitaxy and etching:

```
pdbSet LKMC Post.Epi.Mesh.Update false
```

- The surface produced by LKMC simulation might have many small features and details that, when transferred, can make it difficult to produce a finite-element mesh especially in three dimensions. In some situations such as thin gaps between the epi layer and the existing structure, or if there are sharp features in the grown layer, it is possible to avoid this problem by performing cleanup steps as follows:

To perform cleanup steps before the 3D mesh is created, the following Tcl procedures have been defined:

```
pdbSet LKMC LKMC.Boundary.Proc      <procedure_name>
pdbSet LKMC Combined.Boundary.Proc <procedure_name>
```

Cleanup steps can be performed either directly on the LKMC epitaxy boundary before insertion into the full structure by setting `LKMC.Boundary.Proc` or on the combined structure after the new layer has been inserted using `Combined.Boundary.Proc`. Depending on the situation or problem to be resolved, either procedure or both procedures might be more effective. For example:

```
pdbSet LKMC LKMC.Boundary.Proc cleanLKMC
pdbSet LKMC Combined.Boundary.Proc cleanCombined

proc cleanLKMC { } {
    grid smooth.brep \
        set.repair.resolution=5.e-4 \
        set.delpsc.resolution=5.e-4 \
        set.delpsc.accuracy=5.e-5
    grid brep.stats
    struct tdr.bnd= smoothLKMC
}

proc cleanCombined { } {
    array set stats [grid brep.stats]
    set mda $stats(brep.min.dihedral.angle)
    LogFile "Min dihedral angle: $mda"

    if { $mda < 5 } {
        LogFile "Smoothing..."
    } else {
        LogFile "Skipping smooth."
```

```
        return
    }

    grid smooth.brep \
        set.repair.resolution=5.e-4 \
        set.delpsc.resolution=5.e-4 \
        set.delpsc.accuracy=5.e-5
    grid brep.stats
    struct tdr.bnd= smoothCombined
}
```

**NOTE** The procedures named in LKMC.Boundary.Proc and Combined.Boundary.Proc must include only operations that modify or query the boundary. Any operations working directly on the bulk mesh will be ineffective (since a mesh is generated immediately after these procedures are called) or might possibly fail.

- You can use the following PDB parameter to further reduce small gaps between the extracted LKMC boundary surface and the existing structure (the parameter is switched off by default):

```
pdbSet LKMC Enhance.Filling 1
```

The finite-element structure is also updated after LKMC etching and after steps where both etching and deposition can occur (see [Etching on page 601](#)).

---

## Updating a PDE Structure During Epitaxy in Nonatomistic Mode

In nonatomistic mode and with `1kmc` specified in the `diffuse` command, multiple alternating continuum diffusion and LKMC growth substeps are used to simulate the process. If there are many substeps, or the overall epi thickness is thin, each substep can create structures that are so thin they cause meshing to fail.

To prevent such a situation, you have an optional flow that merges regions, creates a mesh, and applies doping after meshing has occurred. In most cases, the merged boundary is much easier to mesh, but the resolution of the doping profile is not guaranteed for this flow. Especially for graded doping, the mesh must be fine enough to capture the required doping profile. To switch on doping before meshing, set the following parameters:

```
pdbSetBoolean LKMC Boundary.Merge.Before.Doping 1
pdbSet Grid Interpolation.Search.Dist 1e-8
```

**NOTE** When using `Boundary.Merge.Before.Doping` with graded doping, it is important to specify a mesh fine enough to capture the doping profile.

---

## Etching

Modeling of chemical vapor etching using Sentaurus Process LKMC is available from within the `Coordinations.Reactions` model (see [Coordinations.Reactions Model on page 576](#)). This capability addresses the addition of etching gases during chemical vapor deposition (CVD) to help with deposition selectivity and the removal of small amounts of deposited material on insulators. Therefore, etching is available from within the `diffuse` command both simultaneously with deposition or independently.

Etching reactions for the `Coordination.Reactions` model are available only when using Advanced Calibration.

**NOTE** Although you can specify custom reactions and ambients for etching, when using the `Coordinations.Reactions` model for both etching and deposition, it is recommended to use the Advanced Calibration set of models (see [Chapter 8 on page 641](#)).

To specify custom ambients and reactions, see [Coordinations.Reactions Model on page 576](#) and [ambient on page 905](#).

As is the case with pure LKMC deposition, the boundary of the material is tracked with a layer of atoms. In the case of deposition, new atoms are added on top, and unused atoms are removed from the bottom. In the case of etching, new atoms are placed in front of the etching surface only in the materials being etched, which currently are Silicon, Germanium, and SiliconGermanium only. If the material is a random alloy, the mole fraction is handled by an appropriate ratio of randomly selected silicon and germanium atoms.

Updating the finite-element structure after etching has the same capabilities and settings as updating the structure after LKMC deposition (see [Updating the Finite-Element Structure During and After Epitaxy on page 598](#)). The only difference is that, for etching, a gas region is inserted into the structure, instead of a material region replacing gas (which is the case for deposition).

In addition, because the `Coordinations.Reactions` model can be used for both etching and deposition simultaneously, depending on the gases and temperatures specified, a count of the total number of atoms deposited and etched is used to determine whether to insert a gas or material region into the finite-element structure.

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However, it is possible that some regions of a structure are etched while others are deposited on. If this is the case, it might be necessary to force the finite-element update module to do both. This is accomplished by specifying:

```
pdbSet LKMC Deposit.PDE.Structure true  
pdbSet LKMC Etch.PDE.Structure true
```

Either command can be specified separately to force the respective insertion type or specified together to ensure both types are considered.

**NOTE** If the amount of boundary movement is small, the finite-element update can produce thin layers that can lead to instabilities in mesh generation. Therefore, it is suggested to force both etching and deposition updates *only* when both etching and deposition boundaries have moved more than 1 nm.

---

## References

- [1] I. Martin-Bragado, *Simulación atomística de procesos para Microelectrónica*, Ph.D. thesis, Universidad de Valladolid, Valladolid, Spain, 2004.
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# Writing Partial Differential Equations Using Alagator

---

*This chapter discusses how to specify partial differential equations and boundary conditions for use in simulations using the Alagator scripting language.*

The partial differential equations (PDEs) are expressed in a Newton iteration-ready form and are specified as strings that are assumed to equal zero. Most mathematical operators are supported, and operators for differential terms are available.

Care must be exercised with the Tcl expansion of variables and strings because, usually, users want variables to be evaluated at runtime, not when they are read.

---

## Available Operators and Variables

The operators and variables of the Alagator scripting language include binary operators, simple functions, differential functions, string names, solution names, subexpressions, constants, and parameters.

---

### Binary and Unary Operators

Most common binary algebraic operators are supported. Unary negation is also supported with the usual mathematical rules applying. [Table 79](#) lists the supported binary and unary operators in order of precedence. Parentheses are supported for grouping operations.

**NOTE** The unary minus (-) and power (^) operators have nonstandard precedence.

Table 79 Precedence of supported binary and unary operators

Operator	Description
-	Unary minus
^	Power; for example, to raise $a$ to the $b$ power, use: $a^b$
*, /	Multiplication, division

## 7: Writing Partial Differential Equations Using Aligator

### Available Operators and Variables

Table 79 Precedence of supported binary and unary operators

Operator	Description
$+, -$	Addition, subtraction
$<, \leq, \geq, >, ==, !=$	Equality, inequality <b>NOTE</b> Care must be used with <i>equals</i> and <i>not equals</i> , since a comparison of floating-point values in this way can be problematic.
$\&\&$	Logical <i>and</i>
$\ $	Logical <i>or</i>
$:$	Conditional operator
$,$	Comma operator for lists

Many comparison operators are implemented. These do not support derivative operations, so they cannot be used with the `grad` operator (see [Differential Functions on page 605](#)). However, they can be used in the `select` command (see [select on page 1168](#)).

Logical operators *and* ( $\&\&$ ) and *or* ( $\|$ ) are provided for use with callback procedures and initialization. When these operators are used as part of a PDE, care must be taken as the Newton method does not ensure convergence for problems that are not first-order continuous.

The conditional operator ( $:$ ) takes three operands:

- The first operand is a condition.
- The second operand is the value of the entire conditional expression if the condition is true.
- The third operand is the value of the entire conditional expression if the condition is false.

**NOTE** When using the conditional operator ( $:$ ), use parentheses around the expressions to ensure the correct order of evaluation.

For example, the command:

```
select z= "(MyData>1e15) ? (1e15) : (MyData)" name= MyData
```

sets the value of `MyData` to  $1\times 10^{15}$  on mesh points where `MyData` is greater than  $1\times 10^{15}$  and does not change `MyData` on mesh points where `MyData` is smaller than  $1\times 10^{15}$ . Since the `select` command works on mesh points, the conditional operator is very useful for truncating profiles.

## Simple Functions

All simple functions take one argument that must be enclosed in parentheses. The argument can be any expression. Most common functions are available, including:

- ‘exp’ natural exponentiation
- ‘log’ natural log
- ‘log10’ log base 10
- ‘sqrt’ square root

In addition, the complementary error function ‘erfc’ and error function ‘erf’ are provided to help build initial doping profiles. All of these functions have supported derivatives and can be used in the specification of PDEs.

The ‘abs’ function and the ‘sign’ function provide an absolute value and a sign operation, respectively. The sign operation returns +1 if the argument is greater than zero and returns -1 if the argument is less than zero. These functions do not provide derivatives and cannot be used as part of a PDE.

---

## Differential Functions

Differential functions are used in PDEs only and are not evaluated with the `select` command. The differential operators are `dt` and `grad`.

Time derivatives are supported with the `dt` operator. It takes a single argument and computes the first-time derivative of the argument for use in a PDE. Time-step integration is provided automatically using the Bank–Rose trapezoidal rule/backward differentiation formula (TRBDF) method [1].

A simple gradient is supported with the `grad` operator. Implied is the evaluation in a discrete sense and the integral around a control volume. For this reason, the divergence (`div`) operator is not required. For example, `A*B*grad(C)` is treated as `div(A*B*grad(C))`.

**NOTE** Sentaurus Process automatically calculates the divergence if the term includes the `grad` operator.

## String Names

Strings that are not recognized as real numbers, operators, or functions are compared to four sets of possible matches:

- The first set is valid solution names created with the `solution` command (see [solution on page 1203](#)).
  - The second set is named subexpressions created with the `term` command (see [term on page 1232](#)).
  - The third set is the data field name.
  - Finally, any remaining strings pass to the Tcl expression function to see whether they can be parsed to a real number constant. This allows parameters from the parameter database to be used in PDEs.
- 

## Solution Names and Subexpressions

Solution names must match exactly the string specified in the `solution name=<c>` command (see [solution on page 1203](#)). This is important because solution names link PDEs to the variables to be solved. Derivatives are taken automatically of all equations with respect to each solution name found in the PDE.

Terms are useful for common subexpressions (see [Using Terms on page 610](#)). The term name used in the PDEs must match exactly the string specified in the `term name=<c>` command (see [term on page 1232](#)).

**NOTE** Terms and data fields with the same name can coexist in a structure. During equation parsing, the term name has higher priority than the data field name for a region.

---

## Constants and Parameters

Anything that does not match the name of a term or solution passes to the Tcl expression parser to see whether it evaluates as a valid expression. The result is treated as a constant. The evaluation of the expression is performed again in the code if the temperature or time changes, so that parameters can have explicit dependencies on these values.

When defining parameters, care must be given to nested declarations. Especially when parameters are derived using the `pdbDelayDouble` command from other parameters, the Tcl expression parser may be unable to expand the entire expression and evaluate it correctly.

For example:

```

pdbSetDouble Si Test Param1 { [Arrhenius 1 2] }           (1)
pdbSetDouble Si Test Param2 { 2.0* [pdbDelayDouble Si Test Param1] } (2)
pdbSetDouble Si Test Param3 { 2.0* [pdbGetDouble Si Test Param1] } (3)
pdbGet Si Test Param2                                     (4)
pdbGet Si Test Param3                                     (5)

```

Lines 1–3 set Param1, Param2, and Param3. Both Param2 and Param3 are derived parameters from Param1. While Param2 uses pdbDelayDouble to obtain the value of Param1, Param3 uses pdbGetDouble. When retrieving data, line 4 will return an error message, and line 5 will return a valid double number without an error message.

The error message is issued because pdbDelayDouble returns an expression of Param1, which is treated as a string by the Tcl expression parser during the evaluation of Param2.

To prevent such errors, Param2 can be encapsulated with the `expr` command, for example:

```
pdbSetDouble Si Test Param2 { [expr 2.0* [pdbDelayDouble Si Test Param1]] }
```

**NOTE** If Sentaurus Process cannot evaluate an expression correctly, it assumes that it is zero.

## Basics of Specifying Partial Differential Equations

In this section, an example is used to illustrate how to specify PDEs using the Alagator scripting language. The general expression for diffusion of species  $C_X$  is given by:

$$\frac{\partial C_X}{\partial t} = \nabla \bullet D \nabla C_X \quad (861)$$

This will be translated to the Alagator language as:

```
ddt (CX) -D*grad (CX) = 0
```

where CX is the solution variable and D is the diffusivity term (see [Using Terms on page 610](#)).

**NOTE** The divergence (`div`) operator is not specified in front of `D*grad (CX)` because it is implied and computed as part of the discretization of PDEs. Whenever the `grad` operator is in a term, it is assumed that the divergence will be taken of that term during assembly.

**NOTE** The argument of the `grad` operator must be a function of the solution variable.

## 7: Writing Partial Differential Equations Using Alagator

### Basics of Specifying Partial Differential Equations

**NOTE** Since the examples in this section use parameters that are not in the parameter database, long-hand `pdbSet` commands are used (see [pdbSet and Related Commands on page 1104](#)).

---

## Building Partial Differential Equations

The simplest diffusion equation uses a constant diffusivity and can be described by Fick's first law and second law. Two main steps are required to initialize and solve this equation:

1. A solution must be defined (see [solution on page 1203](#)).
2. An equation must be entered into the parameter database.

A minimum of two commands can accomplish this, for example:

```
solution name=CX add !negative !damp solve  
pdbSetString Silicon CX Equation "ddt(CX) - \[Arrhenius 0.138 1.37\]*grad(CX)"
```

The first command creates a new solution named `CX` and adds it to the solution list. The solution cannot take negative values, and numeric damping is not applied to the updates of the Newton iteration. The solution must always be solved.

**NOTE** Aliases are defined only for `pdb` commands. The solution name used in PDEs must match exactly the one specified with the `solution` command.

The second command creates an entry in the parameter database for the material `Silicon` and the solution variable `CX`. An entry is made for an `Equation`, which is the predefined entry that Alagator looks for to find a PDE. The string value is the PDE that will be solved for this variable in this material.

In this example, the PDE to be solved is:

```
d(CX)/dt - div(0.138*exp(-1.37/kT)*grad(CX)) = 0
```

Here, `k` is the Boltzmann constant and `T` is the temperature.

**NOTE** The backslash is required for both the opening and closing brackets to prevent immediate evaluation of the Arrhenius function (see [Arrhenius on page 908](#)). The Arrhenius function is a predefined helper function that allows for the simple creation of Arrhenius expressions. It uses the temperature set by the `diffuse` command or the `SetTemp` command (see [SetTemp on page 1188](#)). Since the Arrhenius function is not evaluated immediately, the presence of brackets means that the Arrhenius function is inserted directly into the parameter database

equation and is evaluated *during* the diffusion. For each diffusion time-step, the Arrhenius function will then be evaluated at the current temperature.

---

## Setting the Boundary Conditions

After defining a solution and entering the equation into the parameter database, you need to set boundary conditions.

### Dirichlet Boundary Condition

The previous example can be enhanced by adding a boundary condition to allow in-diffusion of this species from a gas source. For simplicity, it is assumed that the gas source fixes the surface concentration of species CX at  $5 \times 10^{19} \text{ cm}^{-3}$ .

The following commands create this boundary condition, and both commands work on the gas–silicon interface for the CX variable:

```
pdbSetBoolean Gas_Silicon CX Fixed_Silicon 1  
pdbSetString  Gas_Silicon CX Equation_Silicon "CX_Silicon - 5.0e19"
```

The first command indicates that the value will be set on the silicon side (with the \_Silicon option on `Fixed`), that is, a Dirichlet boundary condition will be applied. The keyword `Fixed` is used only with the Dirichlet boundary condition. Fluxes will be ignored at this node and the boundary condition will control the concentration. Specifying `Fixed_Silicon` is critical because there can be three components on any interface: one for each material and one for the interface.

The second command sets the boundary condition equation. The CX variable has `_Silicon` appended to indicate that the concentration of  $5 \times 10^{19} \text{ cm}^{-3}$  is set on the silicon side.

**NOTE** Equations are set to zero by definition.

**NOTE** Interface names are ordered alphabetically. Most interface names are set to the correct order using the `alias` command (for example, `Silicon_Gas` will be interpreted as `Gas_Silicon`). If a new interface name is introduced, the order must be followed.

## 7: Writing Partial Differential Equations Using Aligator

### Basics of Specifying Partial Differential Equations

## Segregation Boundary Condition

If a segregation-type boundary condition is needed, for example, at the oxide–silicon interface, use the following commands:

```
pdbSetString Oxide_Silicon CX Equation_Oxide "(1.6e-7*(CX_Oxide - \
CX_Silicon/0.28))"
pdbSetString Oxide_Silicon CX Equation_Silicon "-(1.6e-7*(CX_Oxide - \
CX_Silicon/0.28))"
```

This boundary condition assumes that an equation for `CX` is solved in the oxide region as well. Otherwise, the equations would be unbalanced at this interface.

Both commands work on the oxide–silicon interface. The `_Silicon` and `_Oxide` options on `Equation` indicate the side of the interface to which the given flux will be applied. The same options on the solution variable `CX` indicate whether the solution variable value at this interface is taken from the oxide side or the silicon side.

**NOTE** The fluxes have opposite signs. The first number ( $1.6 \times 10^{-7}$ ) in the flux equation is the transfer coefficient, and the second number (0.28) is the segregation coefficient.

---

## Using Terms

A *term* is a common subexpression that can be used in multiple instances or to retrieve information. When the term appears in multiple equations, it reduces the maintenance of equations, and the values are easily retrieved from memory and accumulated. The previous example can be modified in the following way (see [term on page 1232](#)):

```
term name= D Silicon eqn= "\[Arrhenius 0.138 1.37\]" store
pdbSetString Silicon CX Equation "ddt(CX) - D * grad(CX)"
```

The first command creates the `D` term, not a local variable. The dollar sign (indicating a Tcl variable) is no longer needed for `D` in the subsequent equation.

The terms are retained until you exit the simulator, so they can be used in other PDEs or in a `select` command (if you want to monitor the diffusivity of `CX`).

To demonstrate the use of terms, you can introduce a new solution variable (`CY`) and the following recombination reaction between `CX` and `CY`:



[Eq. 863](#) states that two species (`CX` and `CY`) annihilate each other when they react.  $K_f$  is the forward reaction rate, and  $CX^*$  and  $CY^*$  are the equilibrium values of the solution variables. The new solution variable is assumed to diffuse according to Fick's law of diffusion.

[Eq. 863](#) can be implemented by the following commands:

```

solution add name=CX !damp !negative solve
solution add name=CY !damp !negative solve

set Kf {[Arrhenius 4.2e-11 0.1]}
set CXStar {[Arrhenius 3.6e27 3.7]}
set CYStar {[Arrhenius 4.0e26 3.97]}

set RCXCY "$Kf * (CX * CY - $CXStar * $CYStar)"

set diff {[Arrhenius 0.138 1.37]}
pdbSetString Silicon CX Equation "ddt(CX) - $diff * grad(CX) + $RCXCY"
set diff {[Arrhenius 0.02 0.3]}
pdbSetString Silicon CY Equation "ddt(CY) - $diff * grad(CY) + $RCXCY"

```

The first two commands create solutions for `CX` and `CY`. The third command is the forward reaction rate. The next two commands set the equilibrium concentrations of `CX` and `CY`. The sixth command sets the `RCXCY` variable to be a subexpression for the recombination reaction. Any excess of `CX` and `CY` is annihilated until the concentrations are at the equilibrium product. Finally, the diffusivity is obtained and the equation is set, similar to the previous example. The recombination reaction is added to both solution variable equations.

A common error is *not* to add reaction terms to all affected equations. When the recombination is positive, it forces the time derivative to become negative to make the equation equal to zero.

Since the `RCXCY` variable is used more than once and may need to be used in other equations, using `terms` is extremely useful. For example:

```

solution add name=CX !damp !negative solve
solution add name=CY !damp !negative solve

set Kf {[Arrhenius 4.2e-11 0.1]}
set CXStar {[Arrhenius 3.6e27 3.7]}
set CYStar {[Arrhenius 4.0e26 3.97]}

term name= RCXCY Silicon eqn= "$Kf * (CX * CY - $CXStar * $CYStar)" store

set diff {[Arrhenius 0.138 1.37]}
pdbSetString Silicon CX Equation "ddt(CX) - $diff * grad(CX) + RCXCY"
set diff {[Arrhenius 0.02 0.3]}
pdbSetString Silicon CY Equation "ddt(CY) - $diff * grad(CY) + RCXCY"

```

This is almost identical to the previous example, except that a term was created. The term can be used in other equations or in a `select` command (if you want to monitor the recombination rates).

## Basics of Specifying Generic Growth Equations

**NOTE** For generic growth equations, most of the definitions are identical to those of diffusion equations. Read [Basics of Specifying Partial Differential Equations on page 607](#) before continuing with this section.

This section provides examples of varying complexity to illustrate how to specify growth equations using the Alagator scripting language.

Consider a reaction where the ambient GX reacts with silicon and forms a new material called TEOS. [Figure 74](#) shows the ambient concentration at each interface and the motion of the growth during the process, where  $J$  represents the fluxes towards the Gas\_TEOS and Silicon\_TEOS interfaces, and the flux of GX inside TEOS.

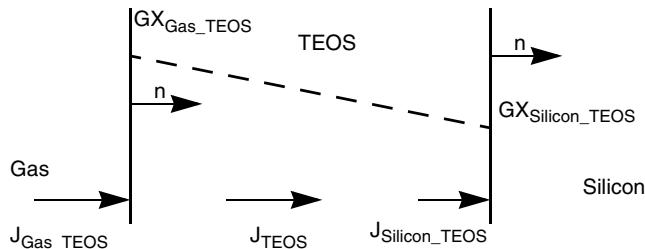


Figure 74 Flux, ambient concentration, and motion of growth front during growth process

Since TEOS is a new material, first, it must be entered into the existing material list using the command:

```
mater add name=TEOS
```

Then, the reacting materials must be defined using the `reaction` command (see [reaction on page 1146](#)).

You can create a reaction based on existing ambients (see [Ambients and Gas Flows on page 647](#)), but in this case, a new react type (named GX) ambient is created:

```
ambient name=GX react add
reaction name=TEOSreaction mat.l=Silicon mat.r=Gas mat.new=TEOS \
new.like=Oxide ambient.name=GX diffusing.species=GX
```

Silicon is the material on the left side (`mat.l`) of the reacting interface, and Gas is the material on the right side (`mat.r`) of the reacting interface. The newly formed material (`mat.new`) at the reacting interface is TEOS. The new material and its interfaces with other materials also are defined to be like Oxide and Oxide interfaces (for example, `TEOS=Oxide`, `PolySilicon_TEOS=Oxide_PolySilicon`) using the `new.like` argument. The GX

reaction requires an ambient, and the ambient name is GX. The reaction will not occur unless the ambient GX is present in a gas flow or directly in the diffuse command. (For more information about how to specify ambients, see [Ambients and Gas Flows on page 647](#).) Reactions that require a react-type ambient cannot have more than one diffusing species name. If the reaction does not require an ambient, it can have multiple names of diffusing species. In this case, the reaction occurs if the reacting interfaces exist in the structure. (This is useful for silicidation.)

The reaction command automatically adds the diffusing species GX to the general solution list. This is performed internally using the following command, where GrowthStep identifies this solution name as a reaction solution name:

```
solution name=GX add !negative GrowthStep solve
```

When the solution name and the new material are defined, the reaction and diffusion equations could be written as follows:

```
pdbSetString TEOS GX Equation "ddt(GX) - \[Arrhenius 0.2 1.86\] *grad(GX) "
pdbSetString Gas_TEOS      GX Equation_TEOS   "-(GX_TEOS - 1e17)"
pdbSetString Silicon_TEOS GX Equation_TEOS   "-5e-2*(GX_TEOS)"
pdbSetString Silicon_TEOS GX GrowthReaction " 5e-2*(GX_TEOS)"
```

The first command sets the diffusion equation of GX in TEOS. The next two commands set the boundary fluxes at the Gas\_TEOS and Silicon\_TEOS interfaces. The \_TEOS option on Equation indicates the side of the interface to which the given flux will be applied. The same option on the solution variable GX indicates that the solution variable value at this interface is taken from the TEOS side. These settings are identical to the ones described in [Setting the Boundary Conditions on page 609](#).

The last command is unique to generic growth equations. The GrowthReaction keyword defines the growth reaction flux at the reacting interface. In this example, the growth reaction flux is identical to the diffusion flux at the reacting interface. In addition, the sign of the growth reaction flux is the opposite of the sign of the diffusion flux.

Finally, you must specify the ambient in a gas flow (see [gas\\_flow on page 964](#)) and use it with the diffuse command, or specify it directly in the diffuse command in order for the reaction to occur. For example, both of these commands will switch on reactions involving the ambient GX and will set the partial pressure of GX to 1:

```
gas_flow name= gxflw partial_pressure= {GX= 1.0}
diffuse time= 100 temp=1000 gas_flow= gxflw
```

or:

```
diffuse time=100 temp=1000 GX
```

## 7: Writing Partial Differential Equations Using Aligator

### Basics of Specifying Generic Growth Equations

Using the `gas_flow` command is more flexible in that the partial pressure can be set to any value (not just 1.0) or the partial pressure can be computed from gas flows and gas reactions.

The model can be enhanced by adding the model parameters to the parameter database. This allows other users to change the values in the equations by accessing the properties directly. The following changes make the equations dependent on the stored value in the parameter database:

```
pdbSetDouble TEOS          GX Dstar "\[Arrhenius 0.2 1.86\]"
pdbSetDouble Gas_TEOS      GX Cstar "1e17"
pdbSetDouble Silicon_TEOS GX Kfd   "5e-2"
pdbSetDouble Silicon_TEOS GX Kfg   "5e-2"

set diff [pdbDelayDouble TEOS GX Dstar]
pdbSetString TEOS GX Equation "ddt(GX) - $diff * grad(GX)"

set GXStar [pdbDelayDouble Gas_TEOS GX Cstar]
pdbSetString Gas_TEOS GX Equation_TEOS "-(GX_TEOS - $GXStar)"

set GKfd [pdbDelayDouble Silicon_TEOS GX Kfd]
pdbSetString Silicon_TEOS GX Equation_TEOS "-$GKfd*(GX_TEOS)"

set GKfg [pdbDelayDouble Silicon_TEOS GX Kfg]
pdbSetString Silicon_TEOS GX GrowthReaction " $GKfg*(GX_TEOS)"
```

The first commands set the diffusivity, the equilibrium value of `GX`, and the forward reaction rates for the diffusion and growth fluxes in the parameter database. The `pdbDelayDouble` command returns the expression stored in the parameter database. This is necessary so that the evaluation of the expression does not occur until the `diffuse` command is executed. Now, the equation depends on the database entry.

The velocities regarding the growth reaction flux are calculated internally as follows:

$$v_{Growth} = \frac{\text{Beta}}{\text{Expansion.Ratio} * \text{Density.Grow}} F_{Growth} \quad (864)$$

where:

- $F_{Growth}$  is the growth reaction flux defined using the `pdbSetString` command and the `GrowthReaction` keyword as previously explained.
- `Beta` is the stoichiometry of the growing material.
- `Expansion.Ratio` is the conversion ratio from consumed material to the growing material.
- `Density.Grow` is the density of the growing material.

The default values for `Beta`, `Expansion.Ratio`, and `Density.Grow` are taken from oxidation of silicon in  $O_2$  ambient.

They are 1, 2.2, and  $2.2 \times 10^{22}$ , respectively, and can be changed using the following commands:

```
pdbSetDouble <interface material> <ambient> Beta <n>
pdbSetDouble <interface material> <ambient> Expansion.Ratio <n>
pdbSetDouble <interface material> <ambient> Density.Grow <n>
```

For the above example, you can change these values with these commands:

```
pdbSetDouble Silicon_TEOS GX Beta 1.1
pdbSetDouble Silicon_TEOS GX Expansion.Ratio 2.0
pdbSetDouble Silicon_TEOS GX Density.Grow 3e22
```

If Expansion.Ratio is set to 0, the material will dissolve but the new material will not form. (For example, silicon will dissolve but no TEOS will form. This is useful for silicidation.)

## Epitaxial Growth

This example uses the reaction command to create a new epitaxial growth mode:

```
ambient name=MyEpi epi add
# Now, create the new temporary material to be used during epi growth
# the name <Ambient>On<Material> is not necessary, it is just
# the same convention as used internally
mater name=MyEpiOnNitride add
reaction name= MyEpiOnNiReact mat.l=Nitride mat.r=Gas mat.new=MyEpiOnNitride \
ambient.name=MyEpi new.like=PolySilicon mat.final=PolySilicon
```

The mat.final argument specifies the name of the final epi material. There is a conversion from mat.new to mat.final at the end of the diffuse command. For details on how to set up epi reactions and growth rates, see [Epitaxy Growth Rate: GrowthRateProc on page 635](#).

## Modifying Built-in Equations and Terms

Sentaurus Process builds equations and terms for known solution variables by default. If you want to add a new expression to an existing equation or term, or to subtract a new expression from an existing equation or term, you can use one of the following commands:

- UserAddEqnTerm
- UserSubEqnTerm
- UserAddToTerm
- UserSubFromTerm
- MultiplyTerm

## 7: Writing Partial Differential Equations Using Aligator

### Modifying Built-in Equations and Terms

**NOTE** Do not use these commands within callback procedures. They are designed to change PDEs without using callback procedures (see [Using Callback Procedures to Build Models on page 618](#)).

**NOTE** All commands except `MultiplyTerm` are saved to TDR files. If the command file is split, the commands must not be included in the new command file. However, if a user-defined variable or term is used with these commands, the variable or term must be included in the new command file, or the variable must be saved with the `define` command (see [define on page 925](#)) and the term must be stored using the `store` argument (see [term on page 1232](#)).

---

## UserAddEqnTerm and UserSubEqnTerm

The `UserAddEqnTerm` and `UserSubEqnTerm` commands allow you to add a new expression to an existing solution variable equation or to subtract the new expression from an existing solution variable equation. The commands have the format:

```
UserAddEqnTerm <material> <solution> <expression> <side> \
    overwrite | !overwrite

UserSubEqnTerm <material> <solution> <expression> <side>
    overwrite | !overwrite
```

where:

- `<material>` is any valid material name.
- `<solution>` is any valid solution variable name.
- `<expression>` is the new expression to be added to or subtracted from the solution variable.
- `<side>` is the side of the interface material where the new expression will be added or subtracted.
- `overwrite | !overwrite` specifies whether or not to overwrite the previous setting. The default is *not* to overwrite (`!overwrite`).

For example, the following command adds the expression " $\{2e-15 * (CY*CY-1e-16*CX)\}$ " to the `CY` equation in silicon by overwriting the previous settings during the PDE solve:

```
UserAddEqnTerm Silicon CY "\{2e-15 * (CY*CY-1e-16*CX)\}" overwrite
```

Since the equations can be set in three different ways for interfaces, you have the option to specify the side to which the expression will be added or subtracted.

For example, the commands:

```
UserAddEqnTerm Oxide_Silicon CX "(CX_Oxide - CX_Silicon)" Silicon
UserSubEqnTerm Oxide_Silicon CX "(CX_Oxide - CX_Silicon)" Oxide
```

add the expression "(CX\_Oxide - CX\_Silicon)" to the Oxide\_Silicon interface equation for CX on the Silicon side, and subtract the same expression from the Oxide\_Silicon interface equation for CX on the Oxide side, respectively. If no side information is given, the expression will be added to the Oxide\_Silicon interface equation for CX.

**NOTE** The UserAddEqnTerm and UserSubEqnTerm commands apply to materials that are *like* the one given with the <material> option.

## UserAddToTerm and UserSubFromTerm

The UserAddToTerm and UserSubFromTerm commands add a new expression to an existing term or subtract the new expression from an existing term. The commands have the format:

```
UserAddToTerm <material> <term> <expression>
UserSubFromTerm <material> <term> <expression>
```

where:

- <material> is any valid material name.
- <term> is an existing term name.
- <expression> is the new expression to be added to or subtracted from the existing term.

For example, the following command adds the expression "2\*CX" to the term MyTerm in silicon:

```
UserAddToTerm Silicon MyTerm "2*CX"
```

In the same way, the following command subtracts the expression "2\*CX" from the term MyTerm in silicon:

```
UserSubFromTerm Silicon MyTerm "2*CX"
```

**NOTE** The UserAddToTerm and UserSubFromTerm commands do not apply to materials that are *like* the one given with the <material> option.

## MultiplyTerm

The `MultiplyTerm` command multiplies a new expression by a user-defined existing term and has the format:

```
MultiplyTerm <material> <term> <expression> [store]
```

where:

- `<material>` is any valid material name.
- `<term>` is an existing term name.
- `<expression>` is the new expression to be multiplied by the existing term.
- `store` specifies that the modified term will be saved to TDR files.

For example, the following command multiplies the expression "2\*CX" by the term `MyTerm` in silicon:

```
MultiplyTerm Si MyTerm "2*CX"
```

**NOTE** By default, the `MultiplyTerm` command is not saved to TDR files. If `MultiplyTerm` is defined with the keyword `store`, the modification of terms is saved to TDR files.

---

## Using Callback Procedures to Build Models

**NOTE** Callback procedures involve complex operations. Only advanced users should use them.

Callbacks allow additional *intelligence* to be built into PDEs by allowing procedures to be called at runtime. These procedures build the Alagator equation strings according to user-specified options. By selecting model switches, you can choose between different physical models to be represented in the equation strings. By having callback procedures that use a material name, a dopant name, or a defect name as arguments, the same type of equation can be built for several materials, dopants, and defect species.

In Sentaurus Process, all frequently used equations are built-in Tcl callback procedures. Using the `pdbSet` command, you can instruct Alagator to use various callback procedures.

You use specific keywords to create callback procedures. [Table 80](#) lists the callback procedure-related keywords in Alagator.

**Table 80** Keywords used to create callback procedures

Keyword	Description
EquationGrowthProc	Specifies the name of the callback procedure to set up equations for material growth (see <a href="#">Constructing Equation Strings: EquationGrowthProc on page 634</a> ).
EquationInitProc	Specifies the name of the callback procedure to set up the initialization equations (see <a href="#">Constructing Initialization Equation String: EquationInitProc on page 631</a> ).
EquationProc	Specifies the name of the callback procedure to set up the PDEs (see <a href="#">Constructing Equation Strings: EquationProc on page 628</a> ).
GrowthRateProc	Defines the PDEs for epitaxial growth (see <a href="#">Epitaxy Growth Rate: GrowthRateProc on page 635</a> ).
InitGrowth	Specifies the name of the callback procedure that usually resets or deletes existing parameter database equations or terms at the beginning of a diffusion simulation (see <a href="#">Cleaning Up Equation Strings and Terms: InitGrowth on page 632</a> ).
InitProc	Specifies the name of the callback procedure that usually resets or deletes existing parameter database equations or terms at the beginning of a diffusion simulation (see <a href="#">Cleaning Up Equation Strings: InitProc on page 627</a> ).
InitSolve	Specifies the name of the callback procedure to reset or delete existing parameter database equations or terms (see <a href="#">Defining the Initialization Equations: InitSolve on page 631</a> ).

---

## Callbacks During Execution of the `diffuse` Command

In addition to calling the callback procedures at various stages during the execution of a `diffuse` command, Sentaurus Process calls the `diffPreProcess` procedure *before* executing the `diffuse` command and the `diffPostProcess` procedure *after* executing the `diffuse` command. The default behavior is described in [Ion Implantation to Diffusion on page 339](#). [Figure 75 on page 620](#) shows the flowchart of this process.

## 7: Writing Partial Differential Equations Using Aligator

### Using Callback Procedures to Build Models

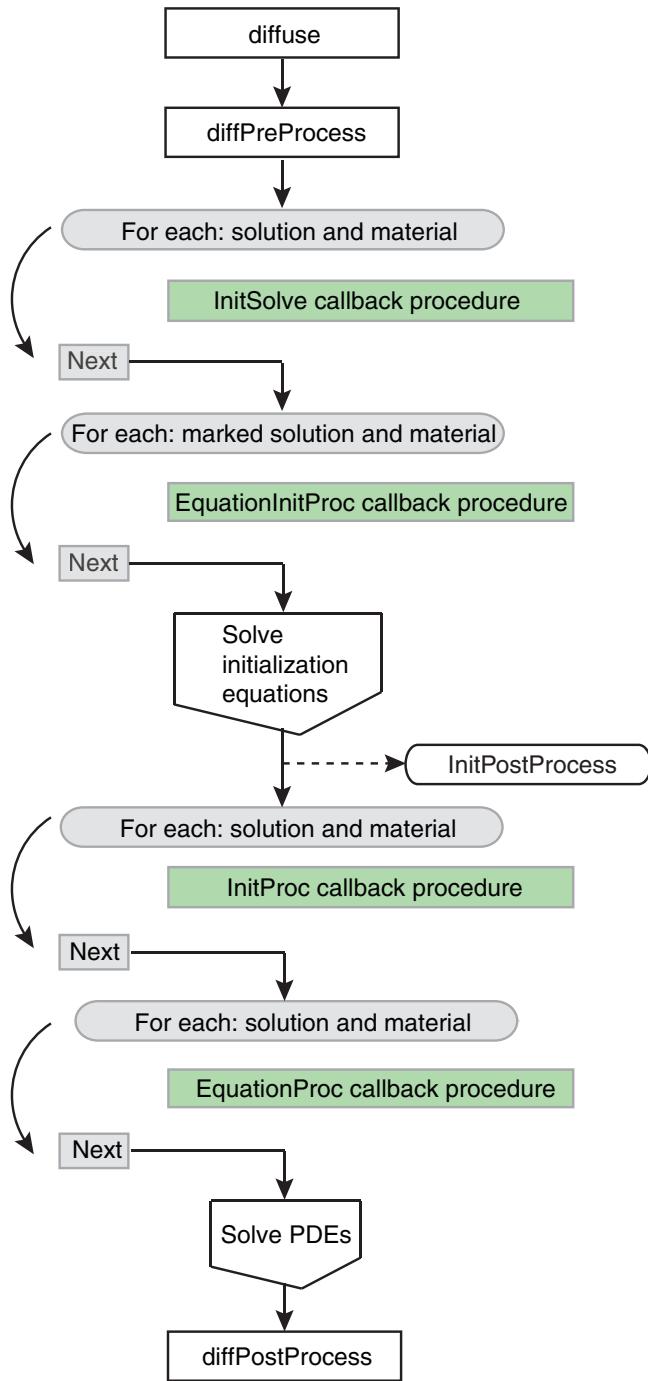


Figure 75 Flowchart with calls to callback procedures during execution of a `diffuse` command

## The diffPreProcess Procedure

Sentaurus Process can initialize solution variable fields on the command line using commands such as `select` (see [select on page 1168](#)) and `profile` (see [profile on page 1137](#)). If the initialization can be standardized, it is better to use the `diffPreProcess` procedure because, by default, it initializes the data fields for interstitials, vacancies, dopants, dopant clusters, dopant-defect clusters, and defect clusters (see [Ion Implantation to Diffusion on page 339](#)).

The execution of each `diffuse` command starts with a call to the `diffPreProcess` procedure that initializes various data fields or preprocesses the existing data fields. For example, the `diffPreProcess` procedure truncates interstitial and vacancy profiles in the amorphous regions. This procedure switches on or off the point-defect equations, the point-defect solutions, and various cluster solutions according to the diffusion models selected.

You can overwrite the `diffPreProcess` procedure. Alternatively, to preserve the preprocessing already implemented in Sentaurus Process, you can implement commands needed for additional preprocessing in the `UserDiffPreProcess` procedure. By default, `UserDiffPreProcess` is an empty procedure and is called from the `diffPreProcess` procedure as one of the last commands.

For example, the following procedure will create a Gaussian profile for the solution variable `CX` with a peak at depth  $x = 0.5$  and a maximum concentration of  $2 \times 10^{18} \text{ cm}^{-3}$ . Ten percent of the `CX` profile will be added to the existing data field `CY`:

```
fproc diffPreProcess { } {
   LogFile "This procedure is used to initialize data fields CX and CY"

    sel z= "CX + 2.0e18 * exp( -(x-0.5)*(x-0.5) / (0.01 * 0.01) ) + 1.0" \
        name= CX store
    sel z= "CY + CX * 0.1" name= CY store
}
```

More complex examples can be created by combining `pdb` commands and callback procedures, for example:

```
pdbSetDouble Silicon CY minDose 1e10

fproc diffPreProcess { } {
   LogFile "This procedure is used to initialize data fields CX and CY"

    sel z = "CX + 2.0e18 * exp( -(x-0.5)*(x-0.5) / (0.01 * 0.01) ) + 1.0" \
        name= CX store
    sel z = CY
    set dose [lindex [integrate] 0]      ;# returns the dose of selected species
                                         ;# (for example, CY) in silicon
    if { $dose > [pdbGetDouble Silicon CY minDose] } {
        solution add name=CY !damp !negative solve
    }
}
```

## 7: Writing Partial Differential Equations Using Aligator

### Using Callback Procedures to Build Models

```
    } else {
        solution add name=CY !damp !negative nosolve
    }
}
```

In this example, the `minDose` parameter is created for `CY` in the parameter database to set the minimum-allowed dose for diffusion to occur. In the `diffPreProcess` procedure, the `CX` profile is set as previously explained. The third and fourth lines calculate the dose of `CY` in silicon. The `if-else` statement returns the minimum dose value from the parameter database. If the existing dose of `CY` is below the minimum dose, the solution for `CY` is switched off; otherwise, it is switched on.

To enforce additional actions to be performed upon diffusion preprocessing, it is not necessary to overwrite the default implementation of the `diffPreProcess` procedure. Instead, to preserve the default initialization of data fields, you can redefine the `UserDiffPreProcess` procedure. By default, `UserDiffPreProcess` is an empty procedure and is called from the `diffPreProcess` procedure as one of the last commands.

## Initialization

After the execution of the `diffPreProcess` procedure, Sentaurus Process checks all material and solution names, and whether a callback procedure has been specified using the `InitSolve` keyword for the material and solution names. If a callback procedure has been defined, this procedure is called using the material name and solution name as arguments (see [Defining the Initialization Equations: InitSolve on page 631](#)).

Subsequently, Sentaurus Process checks all marked materials and solutions to see whether a callback procedure has been specified using the `EquationInitProc` keyword for the solution variable that must be initialized (see [Constructing Initialization Equation String: EquationInitProc on page 631](#)). If this is the case, the callback procedure is executed with the material name and solution name as arguments. Typically, such a callback procedure is used to build the equation string that is solved at `time=0` in the diffusion solver. Alternatively, if no callback procedure has been specified using the `EquationInitProc` keyword, the equation string to be used for the initialization can be specified directly on the command line.

After that, Sentaurus Process solves the initialization equations for all materials and solutions that must be initialized. The initialization equations are solved for the initial temperature of the temperature ramp specified in the `diffuse` command. Such an initialization is usually not required for all solutions. It is typically necessary for solutions whose initial value depends in a complex way on the data fields.

If initialization is not required at all, it can be omitted using `!isolve` in the `diffuse` command.

The Tcl procedure `InitPostProcess` is provided for convenience and is called after the initialization is completed. It can be used to plot or save the solution variable profiles after the initialization. By default, `InitPostProcess` is an empty procedure.

## Building and Solving PDEs

After initialization, Sentaurus Process checks all material and solution names to see whether a callback procedure has been specified using the `InitProc` keyword (see [Cleaning Up Equation Strings: InitProc on page 627](#)). If a callback procedure is defined, it is called for the specified material name and solution name. Such a callback procedure usually sets the equation strings to empty strings and removes terms defined in previous diffusion steps. By having empty equation strings, the equations and terms can be built up piecewise, by adding expressions for each selected model that contributes to an equation or a term. This is necessary because different diffusion models may be used for different diffusion steps, and because additional species may be added between diffusion steps, which may require terms to be added to the equations for existing species.

In the next step, Sentaurus Process checks all material and solution names to see whether a callback procedure has been specified using the `EquationProc` keyword (see [Constructing Equation Strings: EquationProc on page 628](#)). If a callback procedure is defined, it is called with the material name and the solution name as arguments. Such a callback procedure sets the diffusion equations for the solution variable. Alternatively, if no callback procedure is defined for a material and a solution, the equation string can be set on a command line without specifying any callback procedures.

**NOTE** If a callback procedure has been specified using the `EquationProc` keyword for a material name and solution name, this callback procedure typically overwrites any equation specified on the command line for that material and solution.

After the diffusion equations are set, Sentaurus Process solves the equations for the entire temperature cycle specified in the `diffuse` command.

## The `diffPostProcess` Procedure

Finally, the `diffPostProcess` procedure is called at the end of diffusion. It is used mainly to delete data fields that are no longer needed and, by default, it stores the total concentrations of point defects and deletes some temporary data fields such as `Int_Implant` and `Vac_Implant`.

The last command line of the `diffPostProcess` procedure calls the `UserDiffPostProcess` procedure, which is empty by default. To add commands to be executed after diffusion, you can redefine the `UserDiffPostProcess` procedure.

**NOTE** The `diffPreProcess`, `InitPostProcess`, and `diffPostProcess` procedures can be found in the `TclLib` directory in the `DiffProcess.tcl` file (see [Ion Implantation to Diffusion on page 339](#)).

---

## Callbacks During Execution of Generic Growth Equations

**NOTE** This section describes the process for executing the `diffuse` command that includes generic material growth. This section is an extension of [Callbacks During Execution of the `diffuse` Command on page 619](#).

[Figure 76 on page 625](#) shows the flowchart of the execution of a `diffuse` command including generic material growth. The sections regarding diffusion are represented on a smaller scale and are shown in [Figure 75 on page 620](#).

See [Callbacks During Execution of the `diffuse` Command on page 619](#) for descriptions of these various steps and procedures.

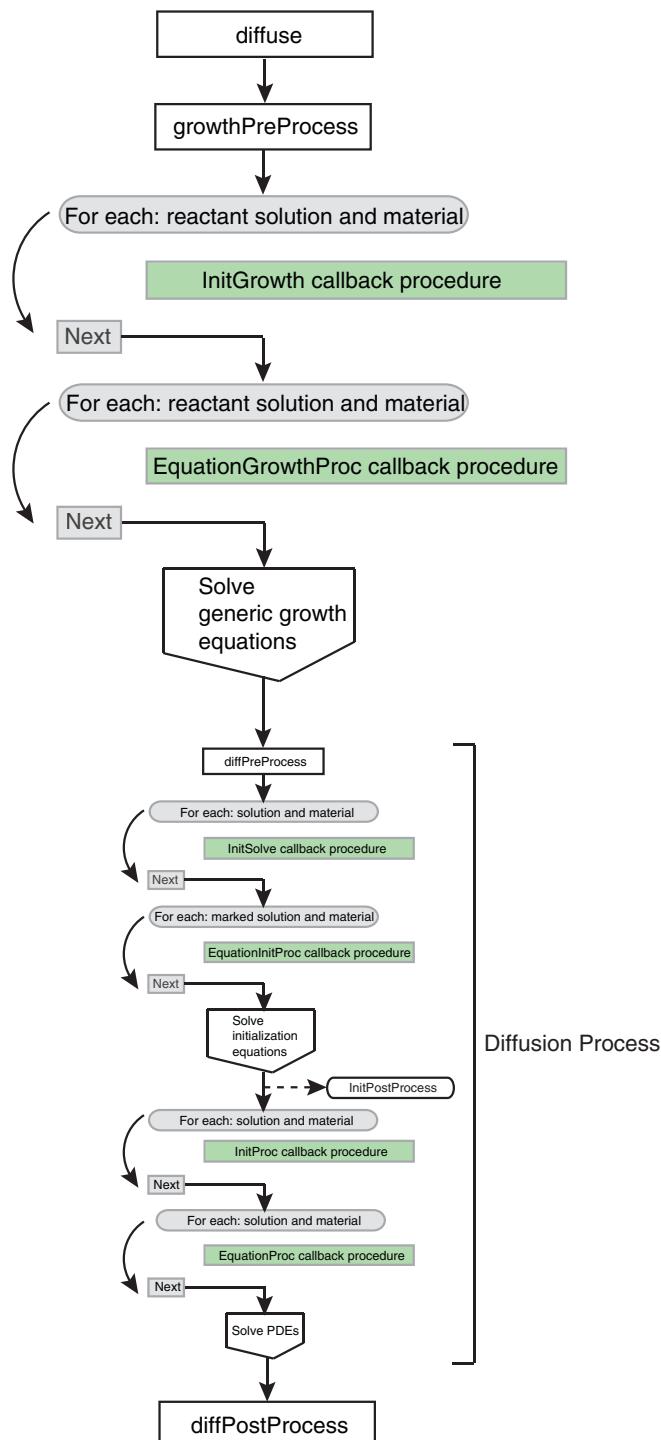


Figure 76 Flowchart with calls to callback procedures during execution of a `diffuse` command, including generic material growth

## 7: Writing Partial Differential Equations Using Aligator

Using Callback Procedures to Build Models

### The growthPreProcess Procedure

The execution of each diffuse command starts with a call to the growthPreProcess procedure that initializes various reaction-related data fields or preprocesses the existing data fields.

To enforce additional actions to be performed upon generic growth preprocessing, it is not necessary to overwrite the default implementation of the growthPreProcess procedure. Instead, to preserve the default initialization of data fields, you can redefine the UserGrowthPreProcess procedure. By default, UserGrowthPreProcess is an empty procedure and is called from the growthPreProcess procedure as one of the last commands.

---

## Specifying Callback Procedures Using Keywords

This section demonstrates how to use keywords to specify callback procedures.

### Common Features of Using Keywords

To avoid unnecessary repetition of content, this section describes common features that apply to all keywords described in the next sections.

Using the `InitProc` keyword as an example, here is a simple demonstration of how you would use this keyword to create a callback procedure:

```
pdbSetString Silicon CX InitProc CleanEquations

proc CleanEquations { Mat Sol } {
   LogFile "This callback procedure unsets $Sol equation in $Mat."
    pdbUnSetString $Mat $Sol Equation
}
```

where:

- The first line specifies the name of the callback procedure in silicon for CX, which follows the keyword instance. In this case, the callback procedure is named `CleanEquations`.
- The second line defines the `CleanEquations` callback procedure.

The callback procedure takes two arguments: a material name (`Mat`) and a solution name (`Sol`). In this example, Sentaurus Process calls the `CleanEquations` procedure with these two arguments: The first will be `Silicon` and the second will be `CX`.

**NOTE** The argument names `Mat` and `Sol` are arbitrary. They can be any valid Tcl variable but the first argument is *always* the material name and the second argument is *always* the solution name.

- The third line defines the message string that will be printed to the log file when the callback procedure is executed. This is to inform users that the callback procedure is called. The \$Sol variable and \$Mat variable will be replaced with the solution name and the material name, respectively. In this case, the message would be:

This callback procedure unsets CX equation in Silicon.

- The fourth and last line unsets the equation if it exists.

## Generic Procedure

When neither the material name nor the solution name is used in the implementation of a callback procedure, it is a *generic* procedure and can be used for several materials and solutions.

The examples in the next sections demonstrate generic procedures.

## Cleaning Up Equation Strings: InitProc

The `InitProc` keyword specifies the name of the callback procedure that cleans up equation strings.

For example, the `InitProc` keyword defines the `ResetEquations` callback procedure of the solution variable `CX` in silicon:

```
pdbSetString Silicon CX InitProc ResetEquations

proc ResetEquations { Mat Sol } {
   LogFile "This callback procedure unsets $Sol equation in $Mat."
    pdbUnSetString $Mat $Sol Equation
}
```

Sentaurus Process will call the `ResetEquations` procedure with two arguments: The first will be `Silicon` and the second will be `CX`.

The procedure is called every time the solutions are checked during the diffusion. The `ResetEquations` procedure prints the message to the log file and removes the parameter database equation if it was defined.

This example can be extended with the following commands:

```
pdbSetString Silicon CX InitProc ResetEquations
pdbSetString Silicon CY InitProc ResetEquations
pdbSetString Oxide   CX InitProc ResetEquations
pdbSetString Oxide   CY InitProc ResetEquations
```

## 7: Writing Partial Differential Equations Using Aligator

### Using Callback Procedures to Build Models

In this case, the same `ResetEquations` callback procedure is used for the solution variables `CX` and `CY` in oxide and silicon. Sentaurus Process will print the following messages:

```
This callback procedure unsets CX equation in Silicon.  
This callback procedure unsets CY equation in Silicon.  
This callback procedure unsets CX equation in Oxide.  
This callback procedure unsets CY equation in Oxide.
```

The advantage of callback procedures is clear. With four new command lines, the equations for `CX` and `CY` in both oxide and silicon can be unset. At the same time, there is only one callback procedure to maintain. If you change the callback procedure, the changes will apply to all four settings.

## Constructing Equation Strings: `EquationProc`

The `EquationProc` keyword specifies the name of the callback procedure that constructs the equation string in the parameter database.

For example, the first command defines `SetEquations` as the callback procedure of the solution variable `CX` in silicon:

```
pdbSetString Silicon CX EquationProc SetEquations  
  
fproc SetEquations { Mat Sol } {  
   LogFile "This callback procedure sets $Sol equation in $Mat."  
    pdbSetString $Mat $Sol Equation "ddt($Sol) - \[Arrhenius 0.138 1.37\] \  
        *grad($Sol)"  
}
```

Sentaurus Process will call `SetEquations` with two arguments: The first will be `Silicon` and the second will be `CX`.

The `SetEquations` callback procedure is called every time the solutions are checked during the simulation. The `SetEquations` procedure prints the message to the log file and sets the parameter database equation for `CX` in silicon.

**NOTE** In this example, the `SetEquations` callback procedure is a generic procedure. The equation setting is similar to that explained in [Building Partial Differential Equations on page 608](#). The only difference is that, instead of using a material name and solution name, only Tcl variables are used.

This example can be extended with the following commands:

```
pdbSetString Silicon CX EquationProc SetEquations  
pdbSetString Silicon CY EquationProc SetEquations
```

In this case, the same `SetEquations` callback procedure is used for the solution variables CX and CY in silicon. Sentaurus Process will print the following messages:

```
This callback procedure sets CX equation in Silicon.  
This callback procedure sets CY equation in Silicon.
```

The above implementation uses the same diffusivity for both CX and CY. To use different diffusivities for each solution variable, the `SetEquations` callback procedure must be modified and diffusivities for each solution variable must be set as follows:

```
pdbSetString Silicon CX EquationProc SetEquations  
pdbSetString Silicon CY EquationProc SetEquations  
  
pdbSetDouble Silicon CX D {[Arrhenius 0.138 1.37]}  
pdbSetDouble Silicon CY D {[Arrhenius 0.02 0.3]}  
  
fproc SetEquations { Mat Sol } {  
    LogFile "This callback procedure sets $Sol equation in $Mat."  
    set diff [pdbDelayDouble $Mat $Sol D]  
    pdbSetString $Mat $Sol Equation "ddt($Sol) - $diff * grad($Sol)"  
}
```

The first change is setting the CX and CY diffusivities in the parameter database. The second change is in the `SetEquations` callback procedure. Instead of having a hard-coded diffusivity number, `pdbDelayDouble` is used to obtain the expression stored in the parameter database. Now, the diffusivities depend on the database entry. You can change these entries to observe the effect of different diffusivities on the final profile.

The example in [Using Terms on page 610](#) can be enhanced by using both terms and callback procedures as follows:

```
pdbSetDouble Silicon CX D {[Arrhenius 0.138 1.37]}  
pdbSetDouble Silicon CY D {[Arrhenius 0.02 0.3]}  
pdbSetDouble Silicon CX Kf {[Arrhenius 4.2e-11 0.1]}  
pdbSetDouble Silicon CY Kf {[Arrhenius 4.2e-11 0.1]}  
pdbSetDouble Silicon CX Cstar {[Arrhenius 3.6e27 3.7]}  
pdbSetDouble Silicon CY Cstar {[Arrhenius 4.0e26 3.97]}  
pdbSetString Silicon CX Recomb "CY"  
pdbSetString Silicon CY Recomb "CX"  
  
solution add name=CX !damp !negative solve  
solution add name=CY !damp !negative solve  
  
pdbSetString Silicon CX EquationProc SetEquations  
pdbSetString Silicon CY EquationProc SetEquations  
  
fproc SetEquations { Mat Sol } {  
    LogFile "This callback procedure sets $Sol equation in $Mat."  
  
    set diff [pdbDelayDouble $Mat $Sol D]
```

## 7: Writing Partial Differential Equations Using Aligator

### Using Callback Procedures to Build Models

```
set Kf    [pdbDelayDouble $Mat $Sol Kf]
set Recomb [pdbGetString $Mat $Sol Recomb]

set CXStar [pdbDelayDouble $Mat $Sol Cstar]
set CYStar [pdbDelayDouble $Mat $Recomb Cstar]

term name= RCXCY $Mat eqn= "$Kf * ($Sol * $Recomb- $CXStar * $CYStar)" store

pdbSetString $Mat $Sol Equation "ddt($Sol) - $diff * grad($Sol) + RCXCY"
}

}
```

First, the diffusivity, the equilibrium concentration, and the forward reaction rate for the recombination of CX and CY are stored in the parameter database. Since CX and CY recombine with each other, this information (Recomb) is also stored in the parameter database. Then, the callback procedure is modified to read these database entries. The Tcl variable `Recomb` in the callback procedure will have the value of CY for CX, and CX for CY. The forward recombination rate `RCXCY` is the same for both solution variables. The callback procedure will be called once for CX and once for CY. During each call, the term `RCXCY` will be created. Since the term name does not depend on the solution name, the first term created during the CX equation setup will be deleted during the CY equation setup. This is performed intentionally, for this example, since both equations use exactly the same term. To create a unique term for each call, the callback procedure must be modified as follows:

```
fproc SetEquations { Mat Sol } {
   LogFile "This callback procedure sets $Sol equation in $Mat."
    set diff [pdbDelayDouble $Mat $Sol D]
    set Kf   [pdbDelayDouble $Mat $Sol Kf]
    set Recomb [pdbGetString $Mat $Sol Recomb]

    set CXStar [pdbDelayDouble $Mat $Sol Cstar]
    set CYStar [pdbDelayDouble $Mat $Recomb Cstar]

    term name = R${Sol}${Recomb} $Mat eqn = "$Kf * ($Sol * $Recomb- $CXStar * \
$CYStar)"

    pdbSetString $Mat $Sol Equation "ddt($Sol) - $diff * grad($Sol) + \
R${Sol}${Recomb}"
}
```

In this case, two terms will be created: `RCXCY` and `RCYCX`.

## Defining the Initialization Equations: InitSolve

In some cases, the initialization of solution variables is very complex and cannot be accomplished using the `select` command. In these cases, Sentaurus Process defines initialization equations using the Alagator language and callback procedures.

Assume that the `CX` solution variable is initialized by solving the following equation:

$$CX_{\text{Total}} = CX + (\alpha CX)^{\beta} \quad (865)$$

where  $CX_{\text{Total}}$  is the total concentration of `CX`, and  $\alpha$  and  $\beta$  are user-defined initialization parameters. Depending on the value of  $\alpha$  and  $\beta$ , you need to solve [Eq. 865](#).

To initiate the initialization setup procedure, the solution name must be defined as:

```
solution add name=CX !damp !negative solve InitStep
```

The option `InitStep` allows this solution variable to be initialized.

The `InitSolve` keyword specifies the name of the callback procedure that Sentaurus Process calls. For example, the first command defines `ResetInitEquations` as the callback procedure of the solution variable `CX` in silicon:

```
pdbSetString Silicon CX InitSolve ResetInitEquations

proc ResetInitEquations { Mat Sol } {
   LogFile "This callback procedure unsets $Sol equation in $Mat during \
        initialization."
    pdbUnSetString $Mat $Sol Equation
}
```

Sentaurus Process will call the `ResetInitEquations` procedure with two arguments: The first will be `Silicon` and the second will be `CX`. The solution variable `CX` is marked to be initialized in silicon. If there is no such setting for the solution variable `CY`, `CY` will not be initialized.

After calling the callback procedures defined by `InitSolve`, Sentaurus Process will look for an equation string for the solution variable. This is performed by defining a callback procedure using the `EquationInitProc` keyword (see [Constructing Initialization Equation String: EquationInitProc](#)).

## Constructing Initialization Equation String: EquationInitProc

The `EquationInitProc` keyword specifies the name of the callback procedure that constructs the equation string for initialization.

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### Using Callback Procedures to Build Models

For example, the first command defines `SetInitEquations` as the callback procedure of the solution variable `CX` in silicon:

```
pdbSetString Silicon CX EquationInitProc SetInitEquations

proc SetInitEquations { Mat Sol } {
    LogFile "This callback procedure sets $Sol equation in $Mat during \
              initialization."
    set alpha [pdbDelayDouble $Mat $Sol Alpha]
    set beta [pdbDelayDouble $Mat $Sol Beta]
    pdbSetString $Mat $Sol Equation "${Sol}_Implant - $Sol - ($alpha * \
              $Sol)^$beta"
}
```

Sentaurus Process will call the `SetInitEquations` procedure with two arguments: The first will be `Silicon` and the second will be `CX`.

**NOTE** The `EquationInitProc` and `EquationProc` keywords work in the same way:

- The callback procedure defined with the `EquationInitProc` keyword is called only during initialization.
- The callback procedure defined with the `EquationProc` keyword is called only during diffusion. It is assumed that `Alpha` and `Beta` are already entered in the parameter database and `CXTotal` is defined.

## Cleaning Up Equation Strings and Terms: `InitGrowth`

**NOTE** The `InitGrowth` keyword is specific to generic growth equations (see [Callbacks During Execution of Generic Growth Equations on page 624](#)).

The `InitGrowth` keyword specifies the name of the callback procedure that cleans up equation strings and terms. For example, the first command defines `ResetEquations` as the name of the callback procedure of the solution variable `GX` in silicon:

```
pdbSetString TEOS GX InitGrowth ResetEquations

proc ResetEquations { Mat Sol } {
    LogFile "This callback procedure unsets $Sol equation in $Mat."
    pdbUnSetString $Mat $Sol Equation
}
```

Sentaurus Process will call the `ResetEquations` procedure with two arguments: The first will be `TEOS` and the second will be `GX`.

The `ResetEquations` callback procedure prints the message to the log file and removes the parameter database equation for `GX` in `TEOS` if it was defined.

This example can be extended with the following commands:

```

pdbSetString TEOS      GX InitGrowth ResetEquations
pdbSetString Gas_TEOS  GX InitGrowth ResetEquations
pdbSetString Silicon_TEOS GX InitGrowth ResetEquations

```

In this case, the same `ResetEquations` callback procedure is used for the solution variables `GX` inside `TEOS`, and at the `Gas_TEOS` and `Silicon_TEOS` interfaces. Sentaurus Process will print the following messages:

```

This callback procedure resets GX equation in TEOS.
This callback procedure resets GX equation in Gas_TEOS.
This callback procedure resets GX equation in Silicon_TEOS.

```

Since the interface equations can be written for the interface material itself or the neighboring materials, all of them must be unset including the growth reaction equation. In this case, you can write a special Tcl procedure for the interfaces as follows:

```

proc ResetInterfaceEquations {Mat Sol} {
    set mater1 [FirstMat $Mat]
    set mater2 [SecondMat $Mat]

    pdbUnSetString $Mat $Sol Equation
    LogFile "This callback procedure resets $Sol equation in $Mat."

    pdbUnSetString $Mat $Sol Equation_$mater1
    LogFile "This callback procedure resets $Sol equation in $Mat on $mater1 \
side."

    pdbUnSetString $Mat $Sol Equation_$mater2
    LogFile "This callback procedure resets $Sol equation in $Mat on $mater2 \
side."

    pdbUnSetString $Mat $Sol GrowthReaction
    LogFile "This callback procedure resets $Sol growth reaction equation in \
$Mat."
}

pdbSetString Gas_TEOS  GX InitGrowth ResetInterfaceEquations
pdbSetString Silicon_TEOS GX InitGrowth ResetInterfaceEquations

```

The `ResetInterfaceEquations` callback procedure is similar to the `ResetEquations` procedure. The commands `FirstMat` and `SecondMat` in the procedure return the names of the neighboring materials (for example, `Gas` and `TEOS` for `Gas_TEOS`). Then, the equations set for either side of the interface or the interface are unset including the generic growth reaction

## 7: Writing Partial Differential Equations Using Aligator

### Using Callback Procedures to Build Models

equation. This special procedure is called for GX at the Gas\_TEOS and Silicon\_TEOS interfaces.

Then, Sentaurus Process will print the following messages:

```
This callback procedure resets GX equation in TEOS.  
This callback procedure resets GX equation in Gas_TEOS.  
This callback procedure resets GX equation in Gas_TEOS on Gas side.  
This callback procedure resets GX equation in Gas_TEOS on TEOS side.  
This callback procedure resets GX growth reaction equation in Gas_TEOS.  
This callback procedure resets GX equation in Silicon_TEOS.  
This callback procedure resets GX equation in Silicon_TEOS on Silicon side.  
This callback procedure resets GX equation in Silicon_TEOS on TEOS side.  
This callback procedure resets GX growth reaction equation in Silicon_TEOS.
```

## Constructing Equation Strings: EquationGrowthProc

**NOTE** The EquationGrowthProc keyword is specific to generic growth equations (see [Callbacks During Execution of Generic Growth Equations on page 624](#)).

Primarily, the EquationGrowthProc keyword specifies the name of the callback procedure that constructs the equation string for the material growth reaction. It uses the keyword EquationGrowthProc in the parameter database.

For example, the first command has the effect that, according to [Figure 76 on page 625](#), Sentaurus Process calls the SetEquations procedure with the arguments TEOS and GX:

```
pdbSetString TEOS GX EquationGrowthProc SetEquations  
  
fproc SetEquations { Mat Sol } {  
   LogFile "This callback procedure sets $Sol equation in $Mat."  
    set diff [pdbDelayDouble $Mat $Sol Dstar]  
    pdbSetString $Mat $Sol Equation "ddt($Sol) -$diff * grad($Sol)"  
}
```

The SetEquations procedure is called every time the solutions are checked during the reaction. This procedure prints the message to the log file and sets the parameter database equation for GX in TEOS.

The equation setting is similar to that explained in [Building Partial Differential Equations on page 608](#). The only difference is that instead of using a solution name and a material name, only Tcl variables are used. Since the interface equations settings are different, this example can be extended with the following commands:

```
pdbSetString Gas_TEOS      GX EquationGrowthProc SetInterfaceEquations  
pdbSetString Silicon_TEOS GX EquationGrowthProc SetInterfaceEquations
```

```
fproc SetInterfaceEquations { Mat Sol } {
    set mater1 [FirstMat $Mat]
    set mater2 [SecondMat $Mat]

    if { [pdbIsAvailable $Mat $Sol Cstar] } {
        set GXStar [pdbDelayDouble $Mat $Sol Cstar]
        pdbSetString $Mat $Sol Equation_$mater2 "-($Sol)_$mater2 - $GXStar"
        LogFile "This callback procedure sets $Sol equation in $Mat on $mater2 \
            side."
    } else {
        set GKfd [pdbDelayDouble $Mat $Sol Kfd]
        pdbSetString $Mat $Sol Equation_$mater2 "-$GKfd*($Sol)_$mater2"
        LogFile "This callback procedure sets $Sol equation in $Mat on $mater2 \
            side."

        set GKfg [pdbDelayDouble $Mat $Sol Kfg]
        pdbSetString $Mat $Sol GrowthReaction " $GKfg*($Sol)_$mater2"
        LogFile "This callback procedure sets $Sol growth reaction equation in \
            $Mat."
    }
}
```

Here, the same `SetInterfaceEquations` callback procedure sets up the interface equations on both the `Gas_TEOS` and `Silicon_TEOS` interfaces. The commands `FirstMat` and `SecondMat` in the procedure return the names of the neighboring materials (for example, `Gas` and `TEOS` for `Gas_TEOS`). The command `pdbIsAvailable` returns true (1) if the `Cstar` value is entered in the parameter database for the given material and solution name. In this example, it returns true for the `Gas_TEOS` interface and false for the `Silicon_TEOS` interface. Using this information and the `if-else` statement, the equations can be set for the `Gas_TEOS` and `Silicon_TEOS` interfaces. Now, the diffusivities, the reaction rates, and the equilibrium values depend on the database entries.

## Epitaxy Growth Rate: GrowthRateProc

**NOTE** The `GrowthRateProc` keyword is specific for epitaxial growth (see [Epitaxial Growth on page 615](#)).

The `GrowthRateProc` keyword specifies the name of the callback procedure that sets the `GrowthReaction` parameter database variable during epitaxial growth. The requirements are similar to `EquationGrowthProc`, except that there can be a different growth rate for each epitaxial ambient. For example:

```
fproc mygrproc { Mat Amb } {
    pdbSetString $Mat $Amb GrowthReaction \
        "[simDelayDouble Diffuse EpiThick]- \
        [pdbDelayDouble $Mat $Amb NativeOffset])/ \
```

## 7: Writing Partial Differential Equations Using Alagator

### Summary

```
        [simDelayDouble Diffuse AnnealStepTime] "
    }

    pdbSet Gas_LTEOnOxide LTE GrowthRateProc mygrproc
```

This example demonstrates some simulation parameters that are available to the `GrowthRateProc` keyword:

- The command `[simDelayDouble Diffuse EpiThick]` retrieves the epi thickness set in the `diffuse` or `temp_ramp` command.
- The command `[pdbDelayDouble $Mat $Amb NativeOffset]` retrieves the native layer offset specified in the `diffuse` command. It is set to the native layer thickness if a native layer was deposited automatically. Otherwise, it is 0.
- The command `[simDelayDouble Diffuse AnnealStepTime]` retrieves the total time of the current `temp_ramp` segment or diffuse time.

If a new material is being deposited that is not a standard Sentaurus Process epi material, you must set the following parameters:

```
pdbSetDouble <mat.new>_Gas <ambient.name> Expansion.Ratio 1.0
pdbSetDouble <mat.new>_Gas <ambient.name> Density.Grow 1.0
```

where:

- `<mat.new>` is the name of the new material being grown.
- `<ambient.name>` is the name of the ambient triggering the growth of `<mat.new>`.

---

## Summary

This section summarizes the use of Alagator to write PDEs and the use of callback procedures.

---

## Diffusion

You have been shown how to set up diffusion equations and boundary equations, and to initialize solution variables. The explained approach is perfectly suitable for a small set of solutions, which can be included in one input file and used. However, expanding and maintaining such a file for new solutions and models would be difficult. Therefore, the implementation of all built-in models in Sentaurus Process is divided into three major parts.

### 1. Parameter Database Entries

All of the default Sentaurus Process model parameters such as diffusivities are stored in the parameter database located in the subdirectory `$SCHOME/Params`. This allows you to examine

the parameters in the Parameter Database (PDB) Browser and to use shorthand pdb commands in your input files. From the earlier example, the following parameters would be stored in the parameter database:

```

pdbSetDouble Silicon CX D      { [Arrhenius 0.138 1.37] }
pdbSetDouble Silicon CY D      { [Arrhenius 0.02 0.3] }
pdbSetDouble Silicon CX Kf     { [Arrhenius 4.2e-11 0.1] }
pdbSetDouble Silicon CY Kf     { [Arrhenius 4.2e-11 0.1] }
pdbSetDouble Silicon CX Cstar  { [Arrhenius 3.6e27 3.7] }
pdbSetDouble Silicon CY Cstar  { [Arrhenius 4.0e26 3.97] }
pdbSetString Silicon CX Recomb "CY"
pdbSetString Silicon CY Recomb "CX"
pdbSetDouble Silicon CX Alpha  { [Arrhenius 1.03103e-17 -0.4] }
pdbSetDouble Silicon CX Beta   {4.0}

```

## 2. Solution Names and Callback Procedures

The names of the solution variables and the names of the callback procedures are stored in the SPROCESS.models file located in the \$SPHOME/TclLib subdirectory. From the earlier example, the following would be stored in the SPROCESS.models file:

```

solution add name=CX !damp !negative solve
solution add name=CY !damp !negative solve

pdbSetString Silicon CX EquationProc SetEquations
pdbSetString Silicon CY EquationProc SetEquations

pdbSetString Silicon CX InitProc ResetEquations
pdbSetString Silicon CY InitProc ResetEquations

pdbSetString Gas_Silicon CY InitProc ResetEquations
pdbSetString Gas_Oxide CX InitProc ResetEquations

pdbSetString Silicon CX InitSolve ResetInitEquations
pdbSetString Silicon CX EquationInitProc SetInitEquations

```

## 3. Model Files

The definition of the diffusion and initialization models are stored in Tcl files located in the \$SPHOME/TclLib subdirectory:

```

fproc UserDiffPreProcess { } {
    LogFile "This procedure is used to initialize data fields CX and CY"

    sel z= "CX + 2.0e18 * exp( -(x-0.5)*(x-0.5) / (0.01 * 0.01) ) + 1.0" \
        name= CXTotal store
    sel z= "CY + CXTotal * 0.1" name= CY store
}

fproc ResetEquations { Mat Sol } {
    LogFile "This callback procedure resets $Sol equation in $Mat."

```

## 7: Writing Partial Differential Equations Using Aligator

### Summary

```
    pdbUnSetString $Mat $Sol Equation
}

fproc SetEquations { Mat Sol } {
    LogFile "This callback procedure sets $Sol equation in $Mat."
    set diff [pdbDelayDouble $Mat $Sol D]
    set Kf   [pdbDelayDouble $Mat $Sol Kf]
    set Recomb [pdbGetString $Mat $Sol Recomb]

    set CXStar [pdbDelayDouble $Mat $Sol Cstar]
    set CYStar [pdbDelayDouble $Mat $Recomb Cstar]

    term name= RCXCY $Mat eqn= "$Kf * ($Sol * $Recomb - $CXStar * $CYStar)" store
    pdbSetString $Mat $Sol Equation "ddt($Sol) - $diff * grad($Sol) + RCXCY"
}

fproc ResetInitEquations { Mat Sol } {
    LogFile "This callback procedure unsets $Sol equation in $Mat during \
        initialization."
    pdbUnSetString $Mat $Sol Equation
}

fproc SetInitEquations { Mat Sol } {
    LogFile "This callback procedure sets $Sol equation in $Mat during \
        initialization."
    set alpha [pdbDelayDouble $Mat $Sol Alpha]
    set beta  [pdbDelayDouble $Mat $Sol Beta]
    pdbSetString $Mat $Sol Equation "${Sol}_Implant - $Sol
        - (($alpha*$Sol)^$beta)"
}
```

---

## Generic Growth

You have been shown how to set up reaction equations and fluxes. The explained approach is perfectly suitable for a small set of solutions, which can be included in one input file and used. However, expanding and maintaining such a file for new solutions and models would be difficult. Therefore, the implementation of all built-in models in Sentaurus Process is divided into three major parts.

### 1. Parameter Database Entries

All of the default Sentaurus Process model parameters such as diffusivities are stored in the parameter database located in the subdirectory \$SCHOME/Params. This allows you to examine the parameters in the PDB Browser and to use shorthand pdb commands in your input files. From the earlier example, the following parameters would be stored in the parameter database:

```
pdbSetDouble TEOS          GX Dstar "\[Arrhenius 0.2 1.86\]"
```

```

pdbSetDouble Gas_TEOS      GX Cstar "1e17"
pdbSetDouble Silicon_TEOS GX Kfd   "5e-2"
pdbSetDouble Silicon_TEOS GX Kfg   "5e-2"

```

## 2. Solution Names and Callback Procedures

The names of the reaction variables, the names of materials, and the names of callback procedures are stored in the `SPPROCESS.models` file located in the `$SPHOME/TclLib` subdirectory. From the earlier example, the following would be stored in the `SPPROCESS.models` file:

```

mater add name=TEOS
reaction name=TEOSreaction mat.l=Silicon mat.r=Gas mat.new=TEOS \
    new.like=oxide diffusing.species=GX ambient
pdbSetString TEOS      GX InitGrowth ResetEquations
pdbSetString Gas_TEOS  GX InitGrowth ResetInterfaceEquations
pdbSetString Silicon_TEOS GX InitGrowth ResetInterfaceEquations
pdbSetString Gas_TEOS  GX EquationGrowthProc SetInterfaceEquations
pdbSetString Silicon_TEOS GX EquationGrowthProc SetInterfaceEquations
pdbSetString TEOS      GX EquationGrowthProc SetEquations

```

## 3. Model Files

The definition of the reaction and initialization models are stored in Tcl files located in the `$SPHOME/TclLib` subdirectory:

```

fproc ResetEquations {Mat Sol} {
   LogFile "This callback procedure resets $Sol equation in $Mat."
    pdbUnSetString $Mat $Sol Equation
}

fproc ResetInterfaceEquations { Mat Sol } {
    set mater1 [FirstMat $Mat]
    set mater2 [SecondMat $Mat]

    pdbUnSetString $Mat $Sol Equation
   LogFile "This callback procedure resets $Sol equation in $Mat."

    pdbUnSetString $Mat $Sol Equation_$mater1
   LogFile "This callback procedure resets $Sol equation in $Mat on $mater1 \
        side."

    pdbUnSetString $Mat $Sol Equation_$mater2
   LogFile "This callback procedure resets $Sol equation in $Mat on $mater2 \
        side."

    pdbUnSetString $Mat $Sol GrowthReaction
   LogFile "This callback procedure resets $Sol growth reaction equation in \
        $Mat."
}

```

## 7: Writing Partial Differential Equations Using Aligator

### References

```
}
```

```
fproc SetEquations { Mat Sol } {
    LogFile "This callback procedure sets $Sol equation in $Mat."
    set diff [pdbDelayDouble $Mat $Sol Dstar]

    pdbSetString $Mat $Sol Equation "ddt($Sol) - $diff * grad($Sol)"
}

fproc SetInterfaceEquations { Mat Sol } {
    set mater1 [FirstMat $Mat]
    set mater2 [SecondMat $Mat]

    if { [pdbIsAvailable $Mat $Sol Cstar] } {
        set GXStar [pdbDelayDouble $Mat GX Cstar]
        pdbSetString $Mat $Sol Equation_$mater2 "-(${Sol}_$mater2 - $GXStar)"
        LogFile "This callback procedure sets $Sol equation in $Mat on $mater2 \
                 side."
    } else {
        set GKfd [pdbDelayDouble $Mat $Sol Kfd]
        pdbSetString $Mat $Sol Equation_$mater2 "-$GKfd*(${Sol}_$mater2)"
        LogFile "This callback procedure sets $Sol equation in $Mat on $mater2 \
                 side."

        set GKfg [pdbDelayDouble $Mat $Sol Kfg]
        pdbSetString $Mat $Sol GrowthReaction " $GKfg*(${Sol}_$mater2)"
        LogFile "This callback procedure sets $Sol growth reaction equation in \
                 $Mat."
    }
}
```

---

## References

- [1] R. E. Bank *et al.*, “Transient Simulation of Silicon Devices and Circuits,” *IEEE Transactions on Electron Devices*, vol. ED-32, no. 10, pp. 1992–2007, 1985.

*This chapter describes the use of Advanced Calibration in Sentaurus Process.*

---

## Overview

Synopsys' Consulting and Engineering is working continually on improving the simulation models and optimizing the model parameters for the latest technology. This effort is based on long-standing experience of model calibration for customers and a comprehensive, growing database of state-of-the-art secondary ion mass spectrometry (SIMS) profiles.

With Advanced Calibration in Sentaurus Process, you have a set of models and parameters that have been calibrated to a broad range of technologies, from power devices to advanced CMOS. With these parameters, you can obtain accurate results for many processes in device fabrication such as ion implantation, dopant diffusion and activation, ultrashallow junction formation, and surface dose loss.

The current release of Sentaurus Process includes two different Advanced Calibration parameter files for continuum simulations. The default Advanced Calibration set of models and parameters targets the simulation of silicon, SiGe, and germanium substrates. For the current release of Sentaurus Process, it is placed in a file named `AdvCal_2017.09.fps`.

An additional parameter file, `AdvCal_SiC_2017.09.fps`, targets process simulation of semiconductor devices based on 4H-SiC. Both these files are located in the directory `$STROOT/tcad/$STRELEASE/lib/sprocess/TclLib/AdvCal`.

The models and parameters of `AdvCal_2017.09.fps` are recommended for all technologies for silicon, SiGe, and germanium substrates. The models have been tested extensively in 1D and 2D simulations, and have proven to be accurate and robust.

Advanced Calibration also is available for Sentaurus Process Kinetic Monte Carlo (see [Advanced Calibration for Sentaurus Process KMC on page 562](#)).

---

## Using Advanced Calibration

Advanced Calibration is the recommended starting point for process simulation of all silicon-based, germanium-based, and 4H-SiC-based devices.

## **8: Advanced Calibration**

### Additional Calibration by Users

To use Advanced Calibration in Sentaurus Process, at the beginning of the command file, insert the line:

```
AdvancedCalibration
```

or:

```
AdvancedCalibration 2017.09
```

This command sources the file `$STROOT/tcad/$STRELEASE/lib/sprocess/TclLib/AdvCal/AdvCal_2017.09.fps`.

The procedure `AdvancedCalibration` has two optional arguments `<version>` and `<material>`. The order of arguments is not important. The allowed values for `<material>` are "Si", "SiGe", "Ge", "4H-SiC", and "SiC". The arguments "Si", "SiGe", and "Ge" as well as no material argument will call the default Advanced Calibration parameter file for Si, SiGe, and Ge materials. The arguments "4H-SiC" and "SiC" will call the Advanced Calibration file for 4H-SiC. For example, the following command will call the Advanced Calibration file for 4H-SiC (`AdvCal_SiC_2017.09.fps`):

```
AdvancedCalibration 2017.09 4H-SiC
```

You can use Advanced Calibration parameters and models from previous releases, for example:

```
AdvancedCalibration 2016.12
```

This command sources the file `$STROOT/tcad/$STRELEASE/lib/sprocess/TclLib/AdvCal/AdvCal_2016.12.fps`.

---

## **Additional Calibration by Users**

Advanced Calibration is based on the assumption that all parameters that are not changed in the parameter files are the Sentaurus Process default parameters. To use the Advanced Calibration file `AdvCal_2017.09.fps`, it must be sourced before the real process description.

You can further increase the accuracy of a certain technology by additional fine-tuning of physical parameters. This must be performed by experienced users with a good understanding of the diffusion models and callback procedures of Sentaurus Process.

The best way to perform this is to put all additional calibration in a user calibration file, for example, `user_calibration.fps`. This file includes all project-specific changes of physical parameters or callback procedures with respect to Advanced Calibration.

In the process simulation file, at the beginning of the process simulation, insert the lines:

```
AdvancedCalibration 2017.09  
source ./user_calibration.fps
```

This method has distinct advantages:

- There is a clear separation between the process flow, which is contained in the Sentaurus Process command file, and the selection of physical models and parameters. During calibration of Sentaurus Process for a specific technology, you can first set up the process flow in the command file of Sentaurus Process and then improve the accuracy of the simulation by making changes only in its parameter file. Conversely, if you want to apply the same models and parameters to a different process, it is only necessary to change the file containing the process flow.
- The Advanced Calibration file is used as a starting point. The user calibration file is usually short and clear. You can see all parameter changes with respect to the original Advanced Calibration at a glance.

**NOTE** For detailed documentation of the contents and physical models included in Advanced Calibration as well as a discussion of its accuracy and limitations, refer to the relevant chapters in the *Advanced Calibration for Process Simulation User Guide*.

To accelerate process simulation for power technologies, use the procedures `AdvancedPowerDeviceMode` and `AdvancedPowerDeviceModeReset`. For details, see the *Advanced Calibration for Process Simulation User Guide*.

## **8: Advanced Calibration**

Additional Calibration by Users

*This chapter describes the oxidation and silicidation models available in Sentaurus Process.*

---

## Oxidation

Sentaurus Process can simulate the thermal oxidation of silicon. Due to the conversion ratio from Si to  $\text{SiO}_2$  being greater than one, a new *volume* is generated, which, in turn, leads to the motion of materials and mechanical stress in the structure. The oxidation process has the following steps:

- The diffusion of oxidants ( $\text{H}_2\text{O}$ ,  $\text{O}_2$ ) from the gas–oxide interface through the existing oxide to the silicon–oxide interface.
- The reaction of the oxidant with silicon to form new oxide<sup>1</sup>.
- The motion of materials due to the volume expansion, which is caused by the reaction between silicon and oxide.

The oxidant diffusion equation is solved using the generic partial differential equation (PDE) solver of Sentaurus Process. The simulation of thermal oxidation has the following requirements:

- The silicon or polysilicon region is in contact with gas or an oxide region, which, in turn, is in contact with gas.
- The `diffuse` command specifies a reactive atmosphere.

If silicon or polysilicon is in contact with gas at the beginning of a thermal oxidation, an initial oxide layer is created automatically. The default thickness of this layer is 1.5 nm. The thickness of the initial oxide layer is specified in the parameter database by:

```
pdbSet Grid NativeLayerThickness 1.5e-7
```

This parameter controls the native layer thickness for oxidation and silicidation.

**NOTE** The value of `NativeLayerThickness` must be greater than the value of `Grid Remove.Dist`. Otherwise, Sentaurus Process will reset the value to  $1.5 \times \text{Remove.Dist}$  in one and two dimensions, or it will remove entire native oxide regions in three dimensions.

---

1. In this chapter, *oxide* refers to  $\text{SiO}_2$ .

## 9: Oxidation and Silicidation

### Oxidation

There are several ways to specify a reactive atmosphere. Furthermore, temperature can vary during oxidation, and the ambient can contain contributions from different oxidants. The following sections describe how to handle these cases using Sentaurus Process.

**NOTE** Oxidation occurs in conjunction with mechanics. For information about the mechanical equations, boundary conditions, and material models, see [Chapter 10 on page 677](#).

---

## Basic Oxidation

The `diffuse` command specifies two reactive ambients for oxidation, either `H2O` or `O2`. The oxidation temperature and time must be given. The following example specifies a simple oxidation using a wet ambient temperature at 1000°C for 10 minutes:

```
diffuse temperature=1000<C> time=10<min> H2O
```

A simple temperature ramp can be specified directly in the `diffuse` command using the `ramprate` argument, which sets the change in the temperature over time. The following example specifies a dry oxidation of 10 minutes that starts at 1000°C and ends at 1100°C:

```
diffuse temperature=1000<C> time=10<min> O2 ramprate=10<C/min>
```

**NOTE** The value of `ramprate` can be negative if the temperature must decrease.

---

## Temperature Cycles

The second example in [Basic Oxidation](#) also can be specified using the `temp_ramp` command, for example:

```
temp_ramp name=MyTempRamp temperature=1000 time=10 O2 ramprate=10<C/min>
diffuse temp_ramp=MyTempRamp
```

The first command creates a temperature ramp with the given conditions, and the second command specifies a diffusion referring to this temperature ramp.

To describe more complex temperature cycles within one `diffuse` command, you can use multiple instances of the `temp_ramp` command. A temperature ramp can consist of several segments and, for each segment, one `temp_ramp` command is required. In addition, segments can be grouped using the same name for each segment. For example, a ramp-up, plateau, and ramp-down can be specified as:

```
temp_ramp name=MyCycle temperature=1000<C> time=5<min> H2O ramprate=20<C/min>
temp_ramp name=MyCycle temperature=1100<C> time=10<min> O2
```

```
temp_ramp name=MyCycle temperature=1100<C> time=10<min> ramprate=-10<C/min>
diffuse temp_ramp=MyCycle
```

If you want to set the minimum and maximum reaction/oxidation time steps in minutes globally, for all diffuse commands, specify the following commands:

```
pdbSet Diffuse MinGrowthStep <n>
pdbSet Diffuse MaxGrowthStep <n>
```

See [Parameter Database on page 21](#) for other diffusion-related parameters.

## Ambients and Gas Flows

Sentaurus Process has a flexible scheme for dealing with gas flows. By default, several ambients are available (see [Table 81](#)), and you can create additional ones for new reactions (see [reaction on page 1146](#)).

Table 81 Available ambients

Ambient name	Ambient type	Reactions
O2	react	Oxidation
H2O	react	Oxidation
HCl	inert	Gas reactions only
N2	inert	None
H2	inert	Gas reactions only
Cl2	inert	None
N2O	react	Oxynitridation
NH3	react	Nitridation
Epi	epi	Standard epitaxy
LTE	epi	Low-temperature epitaxy

The react and inert ambients can be specified in any combination using the `gas_flow` command.

The inert ambients are *inert* in the sense that they do not switch on material reactions. However, they can be used in gas flows to change the partial pressure of react ambients through gas reactions or just taking part of the total pressure as is the case with N<sub>2</sub>, for example. As their name implies, the react ambients cause material reactions to occur, such as oxidation.

The epi-type ambients trigger epitaxial growth and must not be used with any other ambient.

## 9: Oxidation and Silicidation

### Oxidation

To specify an ambient is present and to set the partial pressure to 1.0 \* total pressure, you can use the shorthand specification <ambient> in the `diffuse` or `gas_flow` command. Only one ambient can be specified using <ambient>. The pressure argument sets the total pressure and also is available in the `diffuse` or `gas_flow` command. The default total pressure is 1 atm. For epitaxy, specify the appropriate ambient by name.

## Specifying Gas Flows

The `gas_flow` command specifies a mixed gas flow by setting directly either the partial pressures of the gas components or the flow <volume/time>. When a `gas_flow` is specified, it can be referred to from the `temp_ramp` and `diffuse` commands.

The gases present during diffusion can be specified as partial pressures or by using gas flows. When using flow specifications, the partial pressure is computed from gas reactions, the presence of inert gases, and the total pressure. Alternatively, you can specify the partial pressure directly using either `p<ambient>` or `partial.pressure` in the `gas_flow` command. Some examples are:

```
gas_flow name=MyGasFlow pH2O=0.5 pO2=0.5  
gas_flow name=MyGasFlow partial.pressure= {H2O=0.5 O2=0.5}
```

You can also specify the partial pressure directly in the `diffuse` command, for example:

```
diffuse pH2O=0.5 pO2=0.5 temperature=1000 time=10<min>
```

Instead of specifying partial pressures directly, the gas components can be given in terms of flows using the `flow<ambient>` or `flows` argument. Some examples are:

```
gas_flow name=MyGasFlow flowH2O=0.5 flowO2=0.5 flowH2=0.2 flowN2=1.0  
gas_flow name=MyGasFlow flows = {H2O=0.5 O2=0.5 H2=0.2 N2=1.0}
```

If flows are specified, Sentaurus Process calculates the partial pressures of the components assuming a complete reaction of the gases. Because the only effect of inert ambients in Sentaurus Process is to change the partial pressure of reacting ambients, inert ambients must only be set using flows in the `gas_flow` command.

To invoke the gas flow specification as previously given, use:

```
temp_ramp name=MyTempRamp temperature=1000<C> time=10<min> gas_flow=MyGasFlow  
diffuse temp_ramp=MyTempRamp
```

or:

```
diffuse temperature=1000<C> time=10<min> gas_flow=MyGasFlow
```

## Computing Partial Pressures

Given a flow of O<sub>2</sub> in addition to a flow of H<sub>2</sub> or HCl for example, a chemical reaction between the components is taken into account: O<sub>2</sub> is reduced and H<sub>2</sub>O increases. A complete stoichiometric reaction is assumed. The final flows<sup>1</sup> after the reaction are computed in the AmbientReactions procedure as shown in Eq. 866.

If  $\text{flowO}_2\text{init} > 0.5 \cdot \text{flowH}_2\text{init}$ :

$$\begin{aligned}\text{flowO}_2\text{final} &= \text{flowO}_2\text{init} - 0.5 \cdot \text{flowH}_2\text{init} \\ \text{flowH}_2\text{Ofinal} &= \text{flowH}_2\text{Oinit} + \text{flowH}_2\text{init} \\ \text{flowH}_2\text{final} &= 0\end{aligned}\tag{866}$$

else:

$$\begin{aligned}\text{flowO}_2\text{final} &= 0 \\ \text{flowH}_2\text{Ofinal} &= \text{flowH}_2\text{Oinit} + 2 \cdot \text{flowO}_2\text{init} \\ \text{flowH}_2\text{final} &= \text{flowH}_2\text{init} - 2 \cdot \text{flowO}_2\text{init}\end{aligned}\tag{867}$$

In the case where not all of the H<sub>2</sub> is consumed by the reaction, a warning is displayed. If a contribution of HCl is given, the equations read as follows.

If  $\text{flowO}_2\text{init} > \text{flowHClinit}$ :

$$\begin{aligned}\text{flowO}_2\text{final} &= \text{flowO}_2\text{init} - 0.5 \cdot \text{flowHClinit} \\ \text{flowH}_2\text{Ofinal} &= \text{flowH}_2\text{Oinit} + \text{flowHClinit} \\ \text{flowHClfinal} &= 0\end{aligned}\tag{868}$$

else:

$$\begin{aligned}\text{flowO}_2\text{final} &= 0 \\ \text{flowH}_2\text{Ofinal} &= \text{flowH}_2\text{Oinit} + 2 \cdot \text{flowO}_2\text{init} \\ \text{flowHClfinal} &= \text{flowHClinit} - \text{flowO}_2\text{init}\end{aligned}\tag{869}$$

Alternatively, a stoichiometric reaction model for the HCl ambient can be used by setting:

```
pdbSet Diffuse HCl.Reaction.Model Stoichiometric
```

1. The index *init* refers to the initial flows specified by users in the `gas_flow` command, and *final* describes the flow after the chemical reaction.

## 9: Oxidation and Silicidation

### Oxidation

In this case, the equations become the following.

If  $\text{flowO}_2\text{init} > 0.25 \cdot \text{flowHClinit}$ :

$$\begin{aligned}\text{flowO}_2\text{final} &= \text{flowO}_2\text{init} - 0.25 \cdot \text{flowHClinit} \\ \text{flowH}_2\text{O}_{final} &= \text{flowH}_2\text{O}_{init} + 0.5 \cdot \text{flowHClinit} \\ \text{flowHCl}_{final} &= 0 \\ \text{flowCl}_2\text{final} &= 0.5 \cdot \text{flowHClinit}\end{aligned}\tag{870}$$

else:

$$\begin{aligned}\text{flowO}_2\text{final} &= 0 \\ \text{flowH}_2\text{O}_{final} &= \text{flowH}_2\text{O}_{init} + 2 \cdot \text{flowO}_2\text{init} \\ \text{flowHCl}_{final} &= \text{flowHCl}_{init} - 4 \cdot \text{flowO}_2\text{init} \\ \text{flowCl}_2\text{final} &= 2 \cdot \text{flowO}_2\text{init}\end{aligned}\tag{871}$$

The final flows are used internally to compute the partial pressure of each component. Partial pressures are the relevant quantity for the subsequent simulation. These are computed as:

$$p_{Comp} = \text{pressure} \cdot \frac{\text{flow}_{Comp_{final}}}{\sum_{Comp} \text{flow}_{Comp_{final}}}\tag{872}$$

where *Comp* holds for a certain component of the gas mixture, and *pressure* is the total pressure.

### In Situ Steam-Generated Oxidation

Specifying the *in situ* steam-generated (ISSG) option in the `gas_flow` command means that the gas flow condition should be recognized for ISSG oxidation (see [In Situ Steam-Generated Oxidation on page 663](#)). For example:

```
gas_flow name=ISSGflow pressure=12<torr> flowH2=6 flowO2=12 ISSG
```

---

### Oxidant Diffusion and Reaction

For the rigorous simulation of the oxidation process, the dissolution of the oxidant species at the gas–oxide interface, the transport through the existing or already grown oxide, and the consumption at the oxide–silicon interface must be simulated. The dissolution and consumption are modeled by boundary conditions; for the oxidant transport, a diffusion equation is solved in the oxide layer.

The oxidant species H<sub>2</sub>O, O<sub>2</sub>, and N<sub>2</sub>O are defined in the SPROCESS.models file (see [Default Simulator Settings: SPROCESS.models File on page 20](#)) using the reaction command (see [reaction on page 1146](#)):

```
reaction name=dryoxSi mat.l=Silicon mat.r=Gas mat.new=oxide \
    diffusing.species=O2 ambient.name=O2

reaction name=wetoxSi mat.l=Silicon mat.r=Gas mat.new=oxide \
    diffusing.species=H2O ambient.name=H2O

reaction name=n2ooxSi mat.l=Silicon mat.r=Gas mat.new=oxide
    diffusing.species=N2O ambient.name=N2O
```

For mixed oxidant flows, for each species, one diffusion–reaction system is solved. For each oxidant, one dataset is allocated: H<sub>2</sub>O or O<sub>2</sub> or N<sub>2</sub>O [1/cm<sup>3</sup>].

Growth reaction fluxes at the reacting interfaces are defined using the Alagator scripting language (see [Basics of Specifying Generic Growth Equations on page 612](#)). These fluxes are divided internally by the particle density of oxide to obtain the growth velocities. Manipulation of these fluxes is essential for the implementation of empirical growth models, such as the Massoud model, which is not yet covered by a diffusion equation.

For a mixed gas flow, the contributions of both fluxes are summed. At the reaction front, the following reactions are assumed:



The conversion from Si to SiO<sub>2</sub> leads to a volume increase of 125%, which leads to motion and mechanical stresses in the compound.

The oxidant diffusion described by Fick's law leads to the diffusion equation:

$$\frac{\partial c}{\partial t} + \nabla j = 0, \quad \text{where} \quad j = -D\nabla c \quad (874)$$

where  $D$  is the diffusivity of the oxidant and  $j$  is the particle flux.

The flux of oxidants in the normal direction to the surface, going from the gas region to the oxide, is given by:

$$j = h \cdot (c^* - c) \quad (875)$$

where  $h$  is the mass transfer coefficient and  $c^*$  is the solid solubility of the oxidant. If  $h$  is sufficiently large, the concentration of oxidant at the gas–oxide interface is approximately equal to the solid solubility.

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The mass transfer coefficient  $h$  is defined in the parameter database by MassTransfer and is set using the following commands:

```
pdbSet Gas_Oxide O2 MassTransfer <n>
pdbSet Gas_Oxide H2O MassTransfer <n>
pdbSet Gas_Oxide N2O MassTransfer <n>
```

The solid solubility  $c^*$  is a function of the pressure:

$$c^* = p_{Comp} \cdot c_{ref}^* \quad (876)$$

where  $c_{ref}^* = c_{L0} e^{-\frac{(c_{Lw})}{kT}}$  is the reference solid solubility. Its value can be set using the following commands:

```
pdbSet Oxide O2|H2O|N2O CL0 <n>
pdbSet Oxide O2|H2O|N2O CLW <n>
```

where the vertical bar ( $|$ ) represents the logical *or*.

The flux caused by the chemical reaction at the oxidation front is described by:

$$j = \beta k c_{si} \quad (877)$$

The stoichiometry coefficient  $\beta$  is 1 for  $O_2$  and 2 for  $H_2O$ ,  $k$  is the chemical reaction rate, and  $c_{si}$  is the particle density at the oxide–silicon interface. The reaction rate and diffusivity are computed from the linear and parabolic rate constants used in the Deal–Grove model.

## Transition to Linear and Parabolic Rate Constants

Assuming the stationary state in [Eq. 874](#), the growth rate in the 1D case can be described by the Deal–Grove model:

$$\frac{dx_{ox}}{dt} = \frac{B}{2x_{ox} + A} \quad (878)$$

where  $x_{ox}$  describes the thickness of the 1D oxide layer. This equation can be solved analytically. The parabolic rate constant is given by  $B$ , and the linear rate constant is given by  $B/A$ . A deeper analysis reveals relations between the parabolic rate and the diffusivity, and the linear rate and reaction rate. Assuming  $h \gg k$ :

$$D = \frac{\beta B c_{ox}}{2c^*} \quad (879)$$

$$k \approx \frac{c_{ox}(B)}{c^*(A)}$$

where  $C_{ox}$  is the equivalent oxygen concentration in oxide, for example, it is equal to the concentration of H<sub>2</sub>O and one half (1/2) the concentration of O<sub>2</sub>. Both the parabolic rate and the linear rate are functions of pressure and temperature. For the temperature dependency, two Arrhenius functions, for a low-temperature and high-temperature regime, are available:

$$B(T) = \begin{cases} B0.h \cdot \exp\left(-\frac{BW.h}{k_B T}\right), & \text{if } T > BT.\text{break} \\ B0.l \cdot \exp\left(-\frac{BW.l}{k_B T}\right), & \text{else} \end{cases} \quad (880)$$

Taking pressure dependency into account,  $B$  reads:

$$B = B(p, T) = B(T)p_{Comp}^{Bp.\text{dep}/[\text{bar}]} \quad (881)$$

The B0.h, BW.h, B0.l, BW.l, Bp.dep, and BT.break parameters are available in the parameter database in Oxide H<sub>2</sub>O | O<sub>2</sub> | N<sub>2</sub>O.

An equivalent set of equations is solved for the linear rate  $B/A$ :

$$\frac{B}{A}(T) = \begin{cases} BA0.h \cdot \exp\left(-\frac{BAW.h}{k_B T}\right), & \text{if } T > BAT.\text{break} \\ BA0.l \cdot \exp\left(-\frac{BAW.l}{k_B T}\right), & \text{else} \end{cases} \quad (882)$$

The corresponding parameters are BA0.h, BAW.h, BA0.l, BAW.l, BAp.dep, and BAT.break. They are available in the parameter database as follows:

Oxide_Silicon	H <sub>2</sub> O		O <sub>2</sub>		N <sub>2</sub> O	100		110		100
Oxide_PolySilicon	H <sub>2</sub> O		O <sub>2</sub>		N <sub>2</sub> O	100		110		100

They can be set using the pdbSet command, for example:

```
pdbSet O2 110 BA0.h <n>
pdbSet H2O 100 BAT.break <n>)
```

Parameters defining the diffusivity and the parabolic rate constant are *bulk properties* and, therefore, are defined in oxide. Parameters defining the reaction rate and the linear rate constants are *interface properties* and, therefore, are defined on interfaces. This data can also depend on the crystal orientation when crystalline materials are involved.

## Massoud Model

This model is an empirical model that describes an enhanced growth rate in the initial regime of the oxidation. The Massoud model can be seen as an extension of the Deal–Grove model

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### Oxidation

and is in good agreement with measurement. Sentaurus Process uses a slightly different form of the originally suggested model:

$$\frac{dx_{ox}}{dt} = \frac{B}{2x_{ox} + A} + C \exp\left(-\frac{x_{ox}}{L}\right) \quad (883)$$

Here,  $x_{ox}$  is the 1D unmasked oxide thickness. To account for the enhanced growth in the initial regime, the second term of Eq. 883 contributes to the flux (compare with Eq. 878).

Both the  $L$  and  $C$  parameters depend on the crystal orientation and temperature:

$$C(T) = \begin{cases} C0.h \cdot \exp\left(-\frac{CW.h}{k_B T}\right), & \text{if } T > MBAT.break \\ C0.l \cdot \exp\left(-\frac{CW.l}{k_B T}\right), & \text{else} \end{cases} \quad (884)$$

$$L(T) = \begin{cases} L0.h \cdot \exp\left(-\frac{LW.h}{k_B T}\right), & \text{if } T > MBAT.break \\ L0.l \cdot \exp\left(-\frac{LW.l}{k_B T}\right), & \text{else} \end{cases} \quad (885)$$

The parameters `L0.h`, `LW.h`, `L0.l`, `LW.l`, `C0.h`, `CW.h`, `C0.l`, `CW.l`, and `MBAT.break` are available in the parameter database as follows:

```
Oxide_Silicon O2 | H2O | N2O 100 | 110 | 111
Oxide_PolySilicon O2 | H2O | N2O 100 | 110 | 111
```

### Orientation-Dependent Oxidation

For different crystal orientations, you can apply different reaction rates. Internally, Sentaurus Process computes the data fields `Ori100`, `Ori110`, and `Ori111`, which are the coordinates of a unit vector normal to the surface of the material relative to the basis (coordinate system) of the (nonorthogonal) unit vectors (100), (110), and (111) of the crystal.

The surface normal vector is normalized such that  $Ori100 + Ori110 + Ori111 = 1.0$ . Linear interpolation is used to compute the rates on the orientations that do not coincide with the crystallographic directions.

The following constant values are set for these data fields on the interface side of materials, which are marked as amorphous in the parameter database using `<material> Amorphous 1:`

```
Ori100=1.0, Ori110=0.0, Ori111=0.0
```

When saving results in TDR files, these data fields are not stored. However, they can be accessed using the Alagator scripting language. The Tcl procedure `proc OxidantReaction` creates the terms `ReactionRateO2` and `ReactionRateH2O`:

$$k = k_{<100>} \text{Ori100} + k_{<110>} \text{Ori110} + k_{<111>} \text{Ori111} \quad (886)$$

The reaction rates  $k_{<100>}$ ,  $k_{<110>}$ , and  $k_{<111>}$  are computed from the linear rates  $B/A$  given for different orientations. The parameters `L0` and `C` used in the Massoud model depend on the crystal orientation as well.

For information about the TDR format, see the *Sentaurus™ Data Explorer User Guide*.

## Stress-Dependent Oxidation

Stress-dependent oxidation usually refers to the coupling of the oxidant diffusivity and the reaction rate to the local stress field. To handle the stress-dependent oxidant diffusion and stress-dependent reaction rate, two data fields are created internally. The data field `Pressure` is stored by default, but `NStress` is not stored. However, both can be accessed using the Alagator scripting language. The data fields `Pressure` and `NStress` are defined as:

$$\text{Pressure} = -\frac{1}{3}(\sigma_{xx} + \sigma_{yy} + \sigma_{zz}) \quad (887)$$

$$\text{NStress} = -\sum_j \sum_k \sigma_{jk} n_j n_k \quad (888)$$

The components of the stress tensor are given by  $\sigma_{jk}$  and the normal vector at the reaction front is given by  $n_j$ . The definition of `NStress` is only meaningful at an interface.

If either:

```
pdbSetBoolean Oxide Oxidant Stress.Dependent.Growth 1
```

or:

```
pdbSet Oxide_PolySilicon H2O | O2 | N2O Stress.Dependent.Growth 1
pdbSet Oxide_Silicon H2O | O2 | N2O Stress.Dependent.Growth 1
```

is selected, the reaction rate and the diffusivity are modified in the following ways:

$$k(\text{NStress}, T) = k(T) \cdot \min \left\{ S_{max}, e^{\left( \frac{-\text{NStress} \cdot \nabla k}{k_B T} \right)} \right\} \quad (889)$$

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$$D(\text{Pressure}, T) = D(T) \cdot \min \left\{ S_{max}, e^{\left( -\frac{\text{Pressure} \cdot VD}{k_B T} \right)} \right\} \quad (890)$$

The activation volume  $VD$ , being a bulk property, is defined in  $\text{Oxide O}_2 | \text{H}_2\text{O} | \text{N}_2\text{O}$ . The activation volume  $V_k$  controls the impact of the normal stress at the reaction front and, therefore, is defined on interfaces:

```
Oxide_Silicon | Oxide_PolySilicon O2 | H2O | N2O
```

For example:

```
pdbSet Oxide_Silicon O2 Vk <n>
```

To fully enable stress-dependent reaction rate, use the command:

```
pdbSet Diffuse SDReactionRate 1
```

$S_{max}$  is the maximum stress factor and is used to cap the exponential parts.  $S_{max}$  is defined in  $\text{Oxide O}_2 | \text{H}_2\text{O} | \text{N}_2\text{O}$  as `MaxStressFactor`, for example:

```
pdbSet Oxide O2 MaxStressFactor <n>
```

For improved numeric stability, the exponential part can be approximated by a reciprocal function for a small exponent and a linear function for a large exponent. This option is switched off by default and can be switched on with the following command:

```
pdbSet Mechanics TS4CappedExp 1
```

It replaces the maximum stress factor used to cap the exponential part.

### Trap-Dependent Oxidation

Impurities such as nitrogen and fluorine can be trapped at `Oxide_Silicon` interfaces during oxidation. This will reduce the number of oxidizing sites; therefore, the oxidation rate is reduced. To switch on the trap-dependent oxidation model, use the command:

```
pdbSet <interface_material> <O2 | H2O | N2O> TrapDependent <1 | 0>
```

The list of trapped impurities is given with the command:

```
pdbSet <interface_material> O2 | H2O | N2O TrapList {<trapped_impurity-list>}
```

For example, the following command switches on the trapping flux for nitrogen and fluorine:

```
pdbSet Oxide_Silicon O2 TrapList {Nitrogen Fluorine}
```

The models available for the trapping flux of impurities are Trap and TrapGen.

### Trap Model

The interface Trap model describes the trapping flux of impurities by ignoring the detrapping flux. The total impurity flux at interfaces is the sum of the trapping flux into interfaces and the two-phase segregation. This can be achieved by setting the boundary condition to Trap (see [Boundary Conditions on page 343](#)). For example:

```
pdbSet Oxide_Silicon Nitrogen BoundaryCondition Trap
```

Since the surface reaction rate is proportional to the number of available oxidizing sites, the rate of oxidant consumption at the oxidizing interface is given by:

$$\vec{F} = k_s C_{oi} \left(1 - \frac{\sigma_C}{\sigma_{TCMax}}\right) \vec{n}_i \quad (891)$$

where:

- $k_s$  is the surface recombination rate.
- $C_{oi}$  is the oxidant concentration at the interface.
- $\sigma_C$  and  $\sigma_{TCMax}$  are the impurity trapped density and the maximum trap density, respectively.

The maximum trap density is orientation dependent and can be specified using the following commands:

```
pdbSet <interface_material> <trapped impurity> 100 CMax {<n>}
pdbSet <interface_material> <trapped impurity> 110 CMax {<n>}
pdbSet <interface_material> <trapped impurity> 111 CMax {<n>}
```

### TrapGen Model

The interface TrapGen model calculates the trapping flux and the generation flux of impurities. The generation flux by reaction due to the Gen.Ambient gas is added to the Gen.Material side. For example:

```
pdbSet Oxide_Silicon Nitrogen BoundaryCondition TrapGen
pdbSet Oxide_Silicon Nitrogen Gen.Ambient N20
pdbSet Oxide_Silicon Nitrogen Gen.Material Oxide
```

The generation flux in the interface TrapGen model is calculated by:

$$\vec{F} = \rho v \left(\frac{v}{v_{norm}}\right)^\alpha \vec{n}_i \quad (892)$$

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where:

- $\rho$  is the generation density, which is specified with the Gen.Density parameter.
- $v$  is the reaction velocity.
- $v_{norm}$  is the normalization velocity, which is specified with the Gen.Vnorm parameter.
- $\alpha$  is the power of normalized velocity, which is specified with the Gen.Power parameter.

## Dopant-Dependent Oxidation

A dopant-dependent oxidation rate is incorporated through the electron concentration dependence as:

$$k\left(T, \frac{n}{n_t}\right) = k(T) \cdot lc \quad (893)$$

where:

$$lc = 1 + \gamma_V(C_V - 1) \quad (894)$$

$$\gamma_V = GAMMA0 \times \exp\left(\frac{-GAMMAW}{kT}\right) \quad (895)$$

$$C_V = \frac{1 + C^+\left(\frac{n_i}{n}\right) + C^-\left(\frac{n}{n_t}\right) + C^=\left(\frac{n}{n_t}\right)^2}{1 + C^+ + C^- + C^=} \quad (896)$$

The quantities in Eq. 896 are given by the following formulas:

$$C^+ = \exp\left(\frac{E^+ - E_i}{kT}\right) \quad (897)$$

$$C^- = \exp\left(\frac{E_i - E^-}{kT}\right) \quad (898)$$

$$C^= = \exp\left(\frac{2E_i - E^- - E^=}{kT}\right) \quad (899)$$

$$E^+ = 0.35eV \quad (900)$$

$$E^- = E_g - 0.57eV \quad (901)$$

$$E^{\pm} = E_g - 0.12\text{eV} \quad (902)$$

$$E_i = \frac{E_g}{2} + 0.75 \ln(0.719)kT \quad (903)$$

$$E_g = 1.17 - \frac{(4.73 \times 10^{-4})T^2}{T + 636} \text{ eV} \quad (904)$$

The dependence on carrier concentration is a function of the location along the oxidizing interface.

Dopant-dependent oxidation is switched off by default and can be switched on for O<sub>2</sub> and H<sub>2</sub>O, with:

```
pdbSetBoolean Oxide_Silicon O2 DopantDependentReaction 1
pdbSetBoolean Oxide_Silicon H2O DopantDependentReaction 1
```

In Eq. 895, the quantities GAMMA0 and GAMMAW can be set for O<sub>2</sub> and H<sub>2</sub>O ambients, as follows:

```
pdbSetDouble Oxide_Silicon O2 Gamma0 2360
pdbSetDouble Oxide_Silicon O2 GammaW 1.1

pdbSetDouble Oxide_Silicon H2O Gamma0 2360
pdbSetDouble Oxide_Silicon H2O GammaW 1.1
```

The quantities  $E_g$  and  $E_i$  are defined as procedures called DFactorEg and DFactorEi, each taking a single argument, which is temperature. If you want to overwrite them, use:

```
fproc DFactorEg { temp } {
    # enter the function here
}
```

Finally, Eq. 896 is implemented using the expressions for  $C^+$ ,  $C^0$ ,  $C^-$ , and  $C^{\pm}$ , where  $C^0$  is identically equal to 1. To overwrite them for O<sub>2</sub> and H<sub>2</sub>O ambients, use:

```
pdbSetDoubleArray Oxide_Silicon O2 \
    DopantReactFactor {1 <expr 1> 0 <expr 2> -1 <expr 3> -2 <expr4>}
pdbSetDoubleArray Oxide_Silicon H2O \
    DopantReactFactor {1 <expr 1> 0 <expr 2> -1 <expr 3> -2 <expr4>}
```

## Diffusion Prefactors

The reactant diffusivities can be enhanced or retarded due to various new process conditions. If a new model does not exist to simulate the observed behavior, you might want to multiply

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the existing diffusivity with a prefactor. Sentaurus Process allows diffusivities to be multiplied by user-defined factors. For example, in the case of specified O<sub>2</sub> and H<sub>2</sub>O, these are given by:

```
term name= O2DiffFactor add Oxide eqn= 1.0e18/(1.0*N2ox+1.0e18) store  
term name= H2ODiffFactor add Oxide eqn= 1.0e18/(1.0*N2ox+1.0e18) store
```

The effective diffusivity of O<sub>2</sub> and H<sub>2</sub>O will be multiplied by O2DiffFactor and H2ODiffFactor, respectively. In this example, the diffusivity of both reactants will be a function of the dataset N2ox. See [Chapter 7 on page 603](#) for the definition of terms.

---

## Oxidation With Dielectric on Top

Thermal oxidation of silicon with a dielectric on top can be simulated in Sentaurus Process using an Aligator generic growth script. In addition to the oxidation steps outlined in [Oxidation on page 645](#), there are the following additional steps:

- The diffusion of oxidants (H<sub>2</sub>O, O<sub>2</sub>) from the gas–dielectric interface through the dielectric to the dielectric–oxide interface.

This step involves the dissolution of the oxidant species at the gas–dielectric interface and the oxidant transport in the bulk dielectric.

- The diffusion of oxidants (H<sub>2</sub>O, O<sub>2</sub>) from the dielectric to oxide.

This step is modeled by the boundary condition between the dielectric and the oxide.

Use [SetDielectricOxidationMode on page 1176](#) and [UnsetDielectricOxidationMode on page 1254](#) to switch on or switch off this oxidation mode.

---

## N<sub>2</sub>O Oxidation

In N<sub>2</sub>O oxidation or oxynitridation, nitrogen is trapped at Si–SiO<sub>2</sub> interfaces so that the number of oxidizing sites and, in turn, the oxidation rate are reduced. N<sub>2</sub>O oxidation is performed by specifying N2O in the diffuse command. For the thick oxidation regime (that is, the Deal–Grove model), the parameters for N<sub>2</sub>O oxidation are specified similarly to O<sub>2</sub> or H<sub>2</sub>O. For thin oxidation, the Massoud model is modified by multiplying the nitrogen effect as follows:

$$r_{thin} = C \exp\left(-\frac{x_{ox}}{L}\right) \left(1 - \frac{\sigma_N}{\sigma_{max}}\right) \quad (905)$$

$\sigma_{max}$  can be defined for each of the three available silicon orientations and for polysilicon by specifying the N.Thin.Max values for the N2O ambient. For example:

```
pdbSet Oxide_Silicon      N2O 100 N.Thin.Max {Double {[Arrhenius 1.55e14 0.0]}}
```

```
pdbSet Oxide_PolySilicon N2O 100 N.Thin.Max {Double {[Arrhenius 1.55e14 0.0]}}
```

## SiGe Oxidation

Oxidation in SiGe is modeled in the same way as in silicon. The bulk material parameters for oxidation in SiGe are interpolated from silicon and germanium, depending on the mole fraction of Ge in the bulk SiGe. The interface parameters at the oxide–SiGe interface are interpolated from the oxide–silicon and germanium–oxide interfaces. The interpolation of interface parameters is performed using the mole fraction of Ge on the SiGe side.

A model for silicon and germanium segregation is also available in Advanced Calibration. See the *Advanced Calibration for Process Simulation User Guide*.

## SiC Oxidation

Carbon atoms are generated during SiC oxidation. Some carbon atoms diffuse into oxide and react with diffusing oxidants. The reaction of carbon atoms with oxygen atoms generates carbon oxide (CO). Carbon dioxide (CO<sub>2</sub>) formation requires higher energy than CO formation, so that only CO, which is assumed to evaporate instantly, is accounted for. Some carbon atoms are captured at oxidizing interfaces and reduce the oxidant reaction rate. Although silicon atoms also are generated and diffuse into oxide, it is assumed that the Si–O reaction mainly occurs at SiC–oxide interfaces because Si diffusivity in oxide is very low. Therefore, two-stream, that is, carbon and oxidant diffusion in oxide is taken into account.

The default parameter set is provided for Si-face, that is, (0001) and C-face, that is, (000 $\bar{1}$ ) in both O<sub>2</sub> and H<sub>2</sub>O ambients and for (11 $\bar{2}$ 0) in O<sub>2</sub>:

$$\frac{\partial C_{\text{Ox}}}{\partial t} = \nabla(D_{\text{Ox}}\nabla C_{\text{Ox}}) - k_b C_c \frac{C_{\text{Ox}}}{C_{\text{Ox}}^o} \quad (906)$$

$$\frac{\partial C_c}{\partial t} = \nabla(D_c\nabla C_c) - k_b C_c \frac{C_{\text{Ox}}}{C_{\text{Ox}}^o} \quad (907)$$

$$\frac{\partial \sigma_c}{\partial t} = t(\sigma_{c,\text{max}} - \sigma_c)C_c - eC_{c,\text{max}}\sigma_c \quad (908)$$

where:

- $C_c$  is the carbon concentration in oxide, which is named `CarbonReact`.
- $k_b$  is the reaction rate of a carbon atom and an oxidant.
- $D_c$  is the diffusivity of a carbon atom in oxide.
- $C_{\text{Ox}}$  is the oxidant concentration (O<sub>2</sub> or H<sub>2</sub>O).
- $D_{\text{Ox}}$  is the oxidant diffusivity that is calculated from the parabolic parameter  $B$ .

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- $C_{\text{Ox}}^*$  is the concentration for normalization (the  $\text{C}_{\text{Ox}}$  parameter of the oxidant is used).
- $\sigma_c$  is the captured carbon density at interfaces.
- $t$  is the trapping rate of carbon atoms to the interface ( $\text{cm}^3/\text{s}$ ).
- $e$  is the emission rate of carbon atoms from the interface ( $\text{cm}^3/\text{s}$ ).
- $C_{C, \text{max}}$  is the maximum carbon concentration in oxide.
- $\sigma_{c, \text{max}}$  is the maximum carbon trap density at the interface ( $\text{cm}^{-2}$ ).

$k_b$ ,  $D_C$ ,  $C_{C, \text{max}}$ ,  $t$ ,  $e$ , and  $\sigma_{c, \text{max}}$  are given by, for example:

```

pdbSetDouble Oxide CarbonReact O2 Reaction.Rate <n>
pdbSetDouble Oxide CarbonReact Dstar <n>
pdbSetDouble Oxide CarbonReact CMax <n>
pdbSetDouble Ox_SiC CarbonReact 0001 O2 Trapping.Rate <n>
pdbSetDouble Ox_SiC CarbonReact 0001 O2 Emission.Rate <n>
pdbSetDouble Ox_SiC CarbonReact 0001 CMax <n>

```

At the oxide surface, the incoming fluxes of oxidants and carbon atoms into oxide are expressed by:

$$F_{\text{Ox}} = h(C^* - C_{\text{Ox}}) \quad (909)$$

$$F_C = -k_s C_C \quad (910)$$

where  $k_s$  is the mass transfer rate of carbon atoms:

```
pdbSet Gas_Oxide CarbonReact MassTransfer <n>
```

At the SiC–oxide interface, the incoming fluxes of oxidants and carbon atoms into oxide are modeled by:

$$F_{\text{Ox}} = -k_i \left( 1 - \frac{\sigma_c}{\sigma_{c, \text{max}}} \right) C_{\text{Ox}} \quad (911)$$

$$F_C = r_C F_{\text{Ox}} - \frac{\partial \sigma_c}{\partial t} \quad (912)$$

where:

- $k_i$  is the oxidant reaction rate at the interface, which is calculated from the  $B/A$  value.
- $r_C$  is the ratio of the carbon generation rate to the oxidant reaction rate.  $r_C$  is given by:

```
pdbSetDoubleArray Oxide_SiliconCarbide CarbonReact 0001 O2 Reaction.Factor <n>
```

**NOTE** The parameter interpolation of the arbitrary crystal orientation of polytype crystalline materials is not supported. Therefore, regardless of the surface geometry, uniform crystal orientation is assumed.

## In Situ Steam-Generated Oxidation

The low-pressure combustion of hydrogen–oxygen mixtures is effective in producing high-quality oxides. Combustion-like chemical reactions are initiated over the heated wafer, producing a high density of gas-phase radicals ( $O^-$  and  $OH^-$ ) that react rapidly with silicon. The model for such *in situ* steam-generated (ISSG) oxidation empirically describes the oxidation by the radical  $O^-$ , which dominates typical ISSG oxidation. When the pressure is too low, which means the hydrogen–oxygen mixtures flow too fast, the reactant residence time is too short for chemical activity to occur. However, when the pressure increases over some extent, the oxygen-atom density is localized and decreases rapidly downstream of the flame, so that the narrow reaction zone prevents oxygen atoms from reaching the wafer surface. The oxygen-atom concentration at the wafer surface is modeled by [1]:

$$C^* = C_{max}(p_{H2,flow}) \cdot BPD(\alpha, \beta, P_{max};P) \cdot RRZ(P_{lim};P) \quad (913)$$

$C_{max}(p_{H2,flow})$  calculates the maximum oxygen-atom concentration depending on the partial pressure of hydrogen and the total flow of the hydrogen–oxygen mixtures:

$$flow = flowH_2 + flowO_2 \quad (914)$$

$$p_{H2} = flowH_2 / flow \quad (915)$$

$$C_{max}(p_{H2,flow}) = C_{max}(p_{H2}) \cdot (flow / 1slm)^{C.FLOW.W} \quad (916)$$

$$\begin{aligned} C_{max}(p_{H2}) = & C.H2.L.0 \cdot min(C.H2.Break, p_{H2})^{C.H2.L.W} \\ & + C.H2.H.S \cdot max(p_{H2} - C.H2.Break, 0) \end{aligned} \quad (917)$$

$BPD(\alpha, \beta, P_{max};P)$  determines the profile of the oxygen-atom concentration with a given pressure. The dependence on the pressure is modeled by the beta prime distribution (BPD) as follows:

$$BPD(\alpha, \beta, P_{max};P) = \frac{P_n^{\alpha-1} (1+P_n)^{-\alpha-\beta}}{\left(\frac{\alpha-1}{\beta+1}\right)^{\alpha-1} \left(\frac{\alpha+\beta}{\beta+1}\right)^{-\alpha-\beta}} \quad (918)$$

$$P_n = \frac{\alpha-1}{\beta+1} \cdot \frac{P}{P_{max}} \quad (919)$$

## 9: Oxidation and Silicidation

### Nitridation

where  $\alpha$  and  $\beta$  are specified by the parameters Alpha and Beta, respectively.

The pressure at the peak oxygen-atom concentration,  $P_{max}$ , is modeled as follows:

$$P_{max} = P.\text{Max.H2.0} \cdot p_{H2}^{\frac{P.\text{Max.H2.W}}{P.\text{Max.Flow.0}}} + P.\text{Max.Flow.0} \cdot (\text{flow}/1\text{slm})^{\frac{P.\text{Max.Flow.W}}{P.\text{Max.H2.W}}}$$
 (920)

$RRZ(P_{lim};P)$  defines the rapid reaction zone where the oxygen atoms do not reach the silicon surface:

$$RRZ(P_{lim};P) = \frac{1}{2}erfc(P.\text{Limit.Smooth} \cdot (P - P_{lim})/1\text{torr})$$
 (921)

$$P_{lim} = P.\text{Limit.0} + (P.\text{Limit.A} + P.\text{Limit.B} \cdot e^{-P.\text{Limit.W} \cdot p_{H2}}) \cdot \text{flow}$$
 (922)

The values of the parameters from Eq. 916 through Eq. 922 can be modified by setting:

```
pdbSet Oxide ISSG <parameter> <value>
```

The diffusivity and reaction rates of the oxygen atoms can be modified, respectively, by:

```
pdbSet Oxide ISSG D <value>
pdbSet Oxide_Silicon ISSG Ks <value>
```

The process conditions to invoke the ISSG oxidation are defined in the `diffuse` or `gas_flow` command, for example:

```
diffuse temp=1000 time=1 pressure=12<torr> flowH2=6 flowO2=12 ISSG
```

---

## Nitridation

Nitridation of silicon material injects vacancies, reduces the defects due to high interstitial supersaturation, and enhances vacancy-mediated diffusion of dopants. The vacancy injection model is described in [Surface Recombination Model: Normalized on page 347](#). The nitride is grown by consuming silicon on an exposed silicon surface in an  $\text{NH}_3$  gas environment:

```
diffuse temperature=<n> time=<n> NH3
```

The nitride growth model is the same as the oxidation model. The default parameter values were calibrated with published data [2]. The orientation dependency of nitridation is negligible, so that the same parameter values are applied to all orientations by default.

**NOTE** Due to an absence of data, neither pressure dependency nor Fermi-level dependency is taken into account by default.

## Silicidation

You can define models for new materials and reactions. This capability has been used to define models for the growth of titanium, tungsten, cobalt, and nickel silicides. The following sections describe the kinetics of  $\text{TiSi}_2$  growth, the specification of the model and parameters, and suggestions for modeling other silicides.

### $\text{TiSi}_2$ Growth Kinetics

Titanium silicide is assumed to form when silicon atoms react in the silicide with titanium at the titanium silicide–titanium ( $\text{TiSi}_2\text{--Ti}$ ) interface. The dissolution of silicon and the consumption of titanium lead to the deformation of the material layers in the structure.

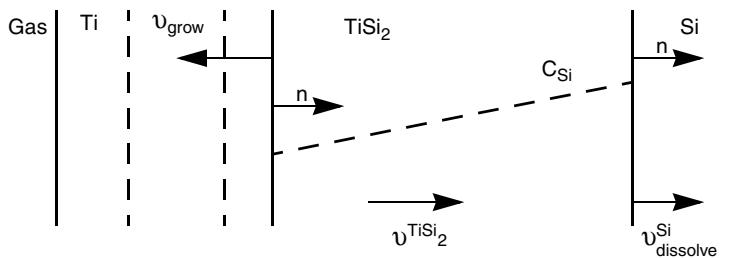


Figure 77 Velocities in 1D silicidation process

**NOTE** While the discussion that follows describes the growth of  $\text{TiSi}_2$  on silicon, it also applies to growth of  $\text{TiSi}_2$  on polycrystalline silicon.

The silicidation process has the following main steps:

- The dissolution of silicon and diffusion of silicon atoms from the  $\text{TiSi}_2$ –silicon interface through the existing  $\text{TiSi}_2$  to the  $\text{Ti}\text{--TiSi}_2$  interface.
- The reaction of silicon with titanium to form new  $\text{TiSi}_2$ .
- The motion of materials due to the volume expansion, which is caused by the reaction between diffused silicon and titanium, and also by the dissolution of silicon at the  $\text{TiSi}_2$ –silicon interface.

**NOTE** The name of the silicide reactant field (which represents the concentration of silicon atoms in the silicide) is `SiliconReact`.

If silicon or polysilicon is in contact with titanium at the beginning of a thermal silicidation, an initial  $\text{TiSi}_2$  layer is created automatically as in the case of oxidation. The default thickness of this layer is 1.5 nm.

## 9: Oxidation and Silicidation

### Silicidation

The thickness of the initial  $\text{TiSi}_2$  layer is specified in the parameter database by:

```
pdbSet Grid NativeLayerThickness 1.5e-7
```

It also controls the native layer thickness for oxidation.

Sentaurus Process automatically recognizes the silicidizing interfaces and switches on the reaction equations.

---

## TiSi<sub>2</sub> Formation Reactions

At the  $\text{TiSi}_2$ –silicon interface, there is the reaction:



where  $Si_{Si}$  is the silicon as a diffusing species on the silicon material side and  $Si_{TiSi_2}$  is the silicon as a diffusing species on the  $\text{TiSi}_2$  material side. Therefore, silicon (on the Si side of the interface) reacts to form silicon atoms (on the  $\text{TiSi}_2$  side of the interface).

The reaction is reversible, allowing for the reformation of silicon (if silicon is released by nitridation of  $\text{TiSi}_2$ , for example):

$$\begin{aligned} R_f &\equiv K_f(C_{Si} - C_{star}) \\ R_g &\equiv \text{Beta } R_f \end{aligned} \quad (924)$$

$R_f$  and  $R_g$  are the diffusion flux and the growth reaction flux, respectively, at the  $\text{TiSi}_2$ –silicon interface. The forward rate of this reaction depends only on temperature, while the reverse rate is also proportional to the concentration of diffusing silicon atoms in  $\text{TiSi}_2$ .  $C_{Si}$  is the concentration of silicon in  $\text{TiSi}_2$ , and  $C_{star}$  is the equilibrium concentration of silicon at the  $\text{TiSi}_2$ –silicon interface. Beta is the stoichiometry of the growing material whose default is 1.0.  $K_f$  is the mass transfer coefficient. To change them, use:

```
pdbSet Silicon_TiSilicide SiliconReact Beta <n>
pdbSet Silicon_TiSilicide SiliconReact Cstar <n>
pdbSet Silicon_TiSilicide SiliconReact Kf <n>
```

For each silicon atom removed from the silicon side of the interface, the volume of silicon is reduced by:

$$\Delta V = \frac{\text{Beta}}{\text{Density.Grow}} \quad (925)$$

where  $\text{Density.Grow}$  is the density of the growing material whose default value is  $5 \times 10^{22}$ .

To change it, use:

```
pdbSet Silicon_TiSilicide SiliconReact Density.Grow <n>
```

There is no new material formation at the  $\text{TiSi}_2$ –silicon interface. Silicon dissolves at this interface and is transported across the  $\text{TiSi}_2$  layer by simple diffusion:

$$\frac{\partial C_{Si}}{\partial t} = \nabla \bullet (D_{star} \nabla C_{Si}) \quad (926)$$

where  $C_{Si}$  is the concentration of silicon in  $\text{TiSi}_2$ , and  $D_{star}$  is the diffusivity of silicon in  $\text{TiSi}_2$ . The following command changes the diffusivity:

```
pdbSet TiSilicide SiliconReact Dstar {<n>}
```

At the  $\text{TiSi}_2$ –titanium interface, there is the reaction:



This reaction is assumed to be irreversible:

$$\begin{aligned} R_f &\equiv K_f(C_{Si} - C_{star}) \\ R_g &\equiv \text{Beta } R_f \end{aligned} \quad (928)$$

$R_f$  and  $R_g$  are the diffusion flux and the growth reaction flux, respectively, at the  $\text{TiSi}_2$ –titanium interface. The reaction rate is proportional to the concentration of diffusing silicon at the  $\text{TiSi}_2$  side of the interface.  $C_{Si}$  is the concentration of silicon in  $\text{TiSi}_2$ , and  $C_{star}$  is the equilibrium concentration of silicon at the titanium– $\text{TiSi}_2$  interface. Beta is the stoichiometry of the growing material whose default is 0.5.  $K_f$  is the mass transfer coefficient. To change them, use:

```
pdbSet TiSilicide_Titanium SiliconReact Beta <n>
pdbSet TiSilicide_Titanium SiliconReact Cstar <n>
pdbSet TiSilicide_Titanium SiliconReact Kf <n>
```

The volumes of titanium and  $\text{TiSi}_2$  change according to:

$$\Delta V = \frac{\text{Beta}}{\text{Expansion.Ratio} * \text{Density.Grow}} \quad (929)$$

where `Expansion.Ratio` is the conversion ratio from consumed material to the growing material (default value is 2.42), and `Density.Grow` is the density of the growing material (default value is  $2.34 \times 10^{22}$ ). These values can be changed using the commands:

```
pdbSet TiSilicide_Titanium SiliconReact Expansion.Ratio <n>
pdbSet TiSilicide_Titanium SiliconReact Density.Grow <n>
```

---

## Tungsten-, Cobalt-, and Nickel-Silicide Models

The tungsten-, cobalt-, and nickel-silicide models are identical in form to the titanium-silicide model. The parameters of the models are different, however, reflecting the differences between the materials (see [3][4] for the tungsten-silicide model and [5][6] for the cobalt-silicide model).

The names of the relevant materials are Tungsten and TungstenSilicide ( $WSi_2$ ), Cobalt and CobaltSilicide ( $CoSi_2$ ), and Nickel and NickelSilicide ( $NiSi$ ).

---

## Multiphase Nickel Silicidation

Besides the fact that nickel silicide ( $NiSi$ ) shows the useful electrical property of low resistivity ( $12\text{--}20 \mu\Omega \cdot \text{cm}$ ), the nickel silicidation process has other advantages such as no line width effect, low Si consumption rate, low film stress, and a low-temperature process. However,  $NiSi$  has multiple phases on which its conductivity strongly depends. Simulating the correct behavior of phase transition during the forming process improves the predictability of the device simulation. The model is invoked by:

```
pdbSet NickelSilicide Multiphase 1 ;# default= 0
```

The model takes the following irreversible reactions, which are energetically favorable [7], into account:  $2Ni + Si \rightarrow Ni_2Si$ ,  $Ni_2Si + Si \rightarrow 2NiSi$ , and  $NiSi + Si \rightarrow NiSi_2$ .

The diffusion equations are:

$$\begin{aligned}\frac{\partial C_{Ni}}{\partial t} &= \nabla \cdot (D_{Ni} \nabla C_{Ni}) - 2k_1 \left( \frac{C_{Ni}}{C_{Ni0}} \right)^2 C_{Si} \\ \frac{\partial C_{Si}}{\partial t} &= \nabla \cdot (D_{Si} \nabla C_{Si}) - k_1 \left( \frac{C_{Ni}}{C_{Ni0}} \right)^2 C_{Si} - k_2 \left( \frac{C_{Ni_2Si}}{C_{Ni_2Si0}} \right) C_{Si} - k_3 \left( \frac{C_{NiSi}}{C_{NiSi0}} \right) C_{Si} \\ \frac{\partial C_{Ni_2Si}}{\partial t} &= k_1 \left( \frac{C_{Ni}}{C_{Ni0}} \right)^2 C_{Si} - k_2 \left( \frac{C_{Ni_2Si}}{C_{Ni_2Si0}} \right) C_{Si} \\ \frac{\partial C_{NiSi}}{\partial t} &= 2k_2 \left( \frac{C_{Ni_2Si}}{C_{Ni_2Si0}} \right) C_{Si} - k_3 \left( \frac{C_{NiSi}}{C_{NiSi0}} \right) C_{Si} \\ \frac{\partial C_{NiSi_2}}{\partial t} &= k_3 \left( \frac{C_{NiSi}}{C_{NiSi0}} \right) C_{Si}\end{aligned}\tag{930}$$

where  $C_{\text{Ni}0}$ ,  $C_{\text{Ni}_2\text{Si}0}$ ,  $C_{\text{NiSi}0}$ , and  $C_{\text{NiSi}_20}$  are the maximum concentrations calculated by the parameter MassDensity and the molecular weight of each silicide by Component information as follows:

```
# Component list
pdbSet NickelSilicide SiliconNiSi Component {Silicon 1}
pdbSet NickelSilicide NickelReact Component {Nickel 1}
pdbSet NickelSilicide Ni2SiReact Component {Nickel 2 Silicon 1}
pdbSet NickelSilicide NiSiReact Component {Nickel 1 Silicon 1}
pdbSet NickelSilicide NiSi2React Component {Nickel 1 Silicon 2}

# Density
pdbSet NickelSilicide NickelReact MassDensity <n>
pdbSet NickelSilicide Ni2SiReact MassDensity <n>
pdbSet NickelSilicide NiSiReact MassDensity <n>
pdbSet NickelSilicide NiSi2React MassDensity <n>
```

$k_1$ ,  $k_2$ , and  $k_3$  are given by the parameter Kf:

```
# Reactions
# 2Ni + Si --> Ni2Si
pdbSet NickelSilicide Ni2SiReact Reactant {NickelReact 2 SiliconNiSi 1}
pdbSet NickelSilicide Ni2SiReact Kf <n>

# Ni2Si + Si --> 2NiSi
pdbSet NickelSilicide NiSiReact Reactant {Ni2SiReact 1 SiliconNiSi 1}
pdbSet NickelSilicide NiSiReact Kf <n>

# NiSi + Si --> NiSi2
pdbSet NickelSilicide NiSi2React Reactant {NiSiReact 1 SiliconNiSi 1}
pdbSet NickelSilicide NiSi2React Kf <n>
```

The boundary conditions at the nickel–NiSi interface are as follows:

$$\begin{aligned}
 F_{\text{Si}} &= -k_{\text{Si}}(C_{\text{Si}} - C_{\text{Si}}^*) \\
 F_{\text{Ni}} &= -k_{\text{Ni}}(C_{\text{Ni}} - C_{\text{Ni}}^*) \\
 F_{\text{Ni}(x)\text{Si}(y)} &= -\frac{r}{\sum yr} F_{\text{Si}} \\
 v_{\text{consumed}} &= \sum x F_{\text{Ni}(x)\text{Si}(y)} \Omega_{\text{Ni}} = -\frac{\Omega_{\text{Ni}} \sum xr}{\sum yr} F_{\text{Si}} = -\frac{\beta}{D \cdot R} F_{\text{Si}} \\
 v_{\text{grow}} &= -\sum F_{\text{Ni}(x)\text{Si}(y)} \Omega_{\text{Ni}(x)\text{Si}(y)} = -\frac{\sum \Omega_{\text{Ni}(x)\text{Si}(y)} r}{\sum yr} F_{\text{Si}} = \frac{\beta}{D} F_{\text{Si}}
 \end{aligned} \tag{931}$$

## 9: Oxidation and Silicidation

### Silicidation

Therefore:

$$D = \beta \cdot \frac{\sum yr}{\sum \Omega_{Ni(x)Si(y)} r} \quad (932)$$

$$R = \frac{\sum \Omega_{Ni(x)Si(y)} r}{\Omega_{Ni} \sum xr}$$

where:

- $\beta$ ,  $D$ , and  $R$  are given by the Beta, Density.Grow, and Expansion.Ratio parameters, respectively.
- $r$  of each NiSi is given by Multiphase.Reaction.Rate.

`Density.Grow` and `Expansion.Ratio` are calculated by the above formula when the  $r$  (`Multiphase.Reaction.Rate`) and the mass density (`MassDensity`) of each silicide are given by the above formula.

- $k_{Si}$  and  $k_{Ni}$  are defined by the parameter `Kf`:

```
pdbSet Nickel_NickelSilicide SiliconNiSi Kf <n>
pdbSet Nickel_NickelSilicide NickelReact Kf <n>
```

- $C_{Si}^*$  and  $C_{Ni}^*$  are given by the parameter `Cstar`:

```
pdbSet Nickel_NickelSilicide SiliconNiSi Cstar <n>
pdbSet Nickel_NickelSilicide NickelReact Cstar <n>
```

- $\Omega_{Ni(x)Si(y)}$  is the atomic or molecular volume of  $Ni(x)Si(y)$ .

Likewise, the boundary conditions at the NiSi–silicon interface are defined.

The `SetMultiphaseNickelSilicide` command sets the values of `Density.Grow` and `Expansion.Ratio` to be consistent with the given parameters `MassDensity` and `Multiphase.Reaction.Rate` (see [SetMultiphaseNickelSilicide on page 1184](#)).

The initial layer of NiSi is filled with 100%  $Ni_2Si$ :

```
pdbSetDoubleArray NickelSilicide Initial.Fields {Ni2SiReact 2.99e22}
```

The volume fraction of each silicide is stored, that is, `Ni2SiFraction`, `NiSiFraction`, and `NiSi2Fraction`. The volume fraction is calculated by:

$$f_{Ni(x)Si(y)} = \frac{\Omega_{Ni(x)Si(y)} C_{Ni(x)Si(y)}}{\sum \Omega_{Ni(x)Si(y)} C_{Ni(x)Si(y)}} \quad (933)$$

**NOTE** The default values of `Kf` and `Multiphase.Reaction.Rate` have not been well calibrated yet.

**NOTE** Unlike other silicidations that remove the react solutions after the silicidation finishes, multiphase nickel silicidation retains the solutions, so that the phases can change during the post-thermal anneal process. In other words, the SiliconNiSi, Ni2SiReact, NiSiReact, and NiSi2React solutions continue to be updated by the post-thermal process even after the silicidation step is completed.

## Stress-Dependent Silicidation

**NOTE** The stress-dependent silicidation model is experimental and can become unstable and can produce irregular shapes. Fundamental changes to the model are possible in future releases.

Similar to oxidation, the silicide reaction rate and the reactant diffusivity can be affected by local stress. For the silicide reaction, the speed of the reaction is assumed to be affected by the total stress energy, so that the stress effect is incorporated symmetrically with respect to tension versus compression.

To switch on stress-dependent silicidation, use the command:

```
StressDependentSilicidation <c>
```

where *<c>* can be set only to NickelSilicide.

When the stress-dependent silicidation model is switched on, the reaction rate given in [Eq. 924](#) and [Eq. 928](#) (that is, at both metal–silicide and silicon–silicide interfaces) is suppressed by the normal stress:

$$K_f(\text{NSTress}, T) = K_f(T) e^{-\left(\frac{\text{abs}(\text{NSTress}) \cdot \text{V}\kappa}{k_B T}\right)} \quad (934)$$

Similarly, the diffusivity of the reactant SiliconReact becomes pressure dependent:

$$D(\text{Pressure}, T) = D(T) e^{-\left(\frac{\text{abs}(\text{Pressure}) \cdot \text{VD}}{k_B T}\right)} \quad (935)$$

The activation volume VD is a bulk property and is defined in the silicide. The activation volume  $\text{V}\kappa$  controls the impact of the normal stress at the reaction front and is defined on interfaces:

```
Nickel_NickelSilicide | NickelSilicide_Silicon
```

For example:

```
pdbSet Nickel_NickelSilicide SiliconReact Vκ <n>
pdbSet NickelSilicide      SiliconReact VD <n>
```

## 9: Oxidation and Silicidation

### Silicidation

In addition to switching on stress dependency of the silicide reaction, the command `StressDependentSilicidation` reduces the viscosity of the silicide to a point where viscous relaxation occurs at typical silicidation temperatures (see [StressDependentSilicidation on page 1215](#)). Similar mass relaxation effects have been proposed in the literature [8][9]. To modify the relaxation of the silicide, use one or both of the following commands:

```
pdbSet NickelSilicide Mechanics Viscosity0 <n>
pdbSet NickelSilicide Mechanics ViscosityW <n>
```

---

## Oxygen-Retarded Silicidation

The silicidation process can be influenced by the presence of oxygen in the silicide. This oxygen is assumed to enter the silicide at interfaces with silicon dioxide and to diffuse in the silicide according to Fick's law. The oxygen retards the reaction of silicon atoms at the silicide–silicon and silicide–metal interfaces and the diffusion of silicon in the silicide. This is called oxygen-retarded silicidation (ORS). The retardation factor is assumed to be in the form of:

$$R_{factor} \equiv 1 - \frac{ORSOxygen}{1 \times 10^{22}} \quad (936)$$

where `ORSOxygen` is the name of the retardant solution. The model can be switched on and off using the command:

```
pdbSet TiSi2 Silicon ORS <0 | 1>
```

If the model is switched on,  $R_{factor}$  is multiplied by  $R_f$  of [Eq. 924, p. 666](#),  $D_{Star}$  of [Eq. 926, p. 667](#), and  $R_f$  of [Eq. 928](#). You can also define the retardation factors using the `term` command with factor terms, for example:

```
term name= SiliconReactReactFactor add TiSilicide /Titanium eqn= \
  "((1-ORSOxygen_TiSilicide/1e22)>0)?(1-ORSOxygen_TiSilicide/1e22):(0.0)" \
  store

term name= SiliconReactDiffFactor add TiSilicide \
  eqn= "((1-ORSOxygen/1e22)>0)?(1-ORSOxygen/1e22):(0.0)" store

term name= SiliconReactReactFactor add Silicon /TiSilicide eqn= \
  "((1-ORSOxygen_TiSilicide/1e22)>0)?(1-ORSOxygen_TiSilicide/1e22):(0.0)" \
  store
```

**NOTE** The oxygen-retarded silicidation model can cause instabilities (such as a zigzag shape of the silicide boundary) because of a high concentration of silicon near the oxide. Solving the silicon diffusion equation in steady-state reduces such instability. It can be switched on using the command:

```
pdbSet NickelSilicide Silicon Steady 1
```

---

## Triple-Point Control

During silicidation, triple points where more than two materials come together (such as oxide, silicon, and silicide node) can move inadvertently due to material consumption around the node. To control the movement, a retardation factor around the triple point is applied to the velocities. The retardation factor is assumed to be:

$$R = \text{Factor} + \frac{2(1 - 2\text{Factor})}{\pi} \tan\left(\frac{SDistance}{Distance}\right) \quad (937)$$

`Factor` is the suppression value at the triple point, and `Distance` is the roll-off length for silicidation triple-point suppression. The distance determines how far the suppression factor will be effective from the triple point. `SDistance` is the distance to the nearest node from the triple point and is calculated internally. The other parameters can be changed using the following commands:

```
pdbSet <material> SilicidationTripleDistance {<n>}  
pdbSet <material> SilicidationTripleFactor {<n>}
```

where `<material>` is the interface material (for example, `Silicon_TiSilicide`). If you want to switch the triple-point control on or off, use the command:

```
pdbSet Mechanics SilicidationCorrection <1 | 0>
```

---

## Dopants and Defects in Oxides and Silicides

Dopants in oxides and silicides are modeled in the same way as in other nonsemiconductor materials. Transport within a silicide or an oxide is governed by simple diffusion (that is, no electric field effects). For details on segregation at material interfaces, see [Boundary Conditions on page 343](#). Point defects can participate in reactions at interfaces with silicon.

While the current oxidation model specifies the generation of interstitials by the consumption of silicon, the current titanium silicide model specifies the generation of vacancies by the same mechanism.

---

## Numerics

During oxidation or silicidation, one material grows at the expense of another material. To handle the growth of materials, Sentaurus Process uses two different time loops – outer and inner – as shown in [Figure 78 on page 674](#) for the case of oxidation.

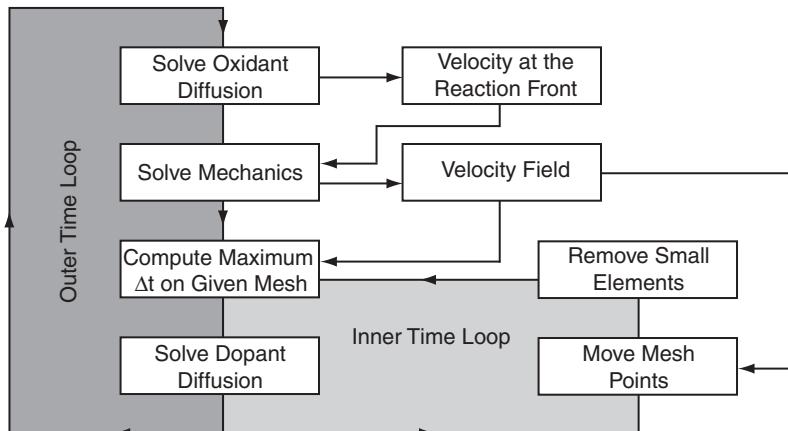


Figure 78 Flowchart for simulation of material growth

## Outer Time Loop

The diffusion equation for the oxidants is solved using the general PDE solver in Sentaurus Process. In addition, a predictor for the next time step (*oxidation time step*) is computed. When the concentrations of oxidants at the oxide–silicon interface are known, the corresponding growth velocities can be computed. These velocities serve as a boundary condition for the mechanics problem. After solving the mechanics problem, the velocity field in the entire structure is known. At this point, the program enters the inner time loop.

## Inner Time Loop

Given a mesh and the velocity field, a time step (*grid time step*) can be computed so that elements do not collapse when applying the velocities to the nodes of the mesh (moving mesh). In the next time step, the dopant diffusion is solved using the general PDE solver and a predictor for the next time step (*diffusion time step*) is computed. Then, mesh points are moved according to the velocity field and, subsequently, small mesh elements are removed.

After removing small elements, the next grid time step is computed. The smaller of the two time steps (grid time step and diffusion time step) is applied in the next time cycle. The inner time loop runs as long as the time step of the outer loop (oxidation time step) is fulfilled. Then, the code goes into its second time step of the outer loop. An example of typical output during oxidation is:

```

...
Reaction Solve from 14.86min to 15.11min. Time step: 15.32s.
Mechanics Solve from 14.86min to 15.11min. Time step: 15.32s.

```

```

Diffusion Solve from 14.86min to 14.99min. Time step: 8.144s.
Diffusion Solve from 14.99min to 15.11min. Time step: 7.176s.
Reaction Solve from 15.11min to 15.37min. Time step: 15.4s.
Mechanics Solve from 15.11min to 15.37min. Time step: 15.4s.
Diffusion Solve from 15.11min to 15.25min. Time step: 8.361s.
Diffusion Solve from 15.25min to 15.29min. Time step: 2.077s.
Diffusion Solve from 15.29min to 15.37min. Time step: 4.967s.
...

```

This output reproduces the following time-stepping scheme:

- Reaction Solve and Mechanics Solve occur in the outer time loop.
- Diffusion Solve occurs in the inner time loop.

As previously mentioned, after solving the mechanics problem, velocities are given on all mesh points. Mesh points are moved according to these velocities. This leads to a change in the geometry and, in some cases, also to a change in the topology of the structure at each time step. At a reactive interface, for example at the oxidation front, two velocities apply: one describes the growth of a material and one describes the consumption of another material.

The velocity describing the growth of the material is used to solve the mechanics problem, and the velocities describing the consumption of a material are used to update the structure or mesh. Therefore, mesh elements on the growing side of the oxidation front are *stretched*, and elements on the shrinking side are *compressed*. Edges on the growing side, which become too long with time, are split. Edges and elements on the shrinking side of the interface that become too small are removed. This is shown in [Figure 79](#).

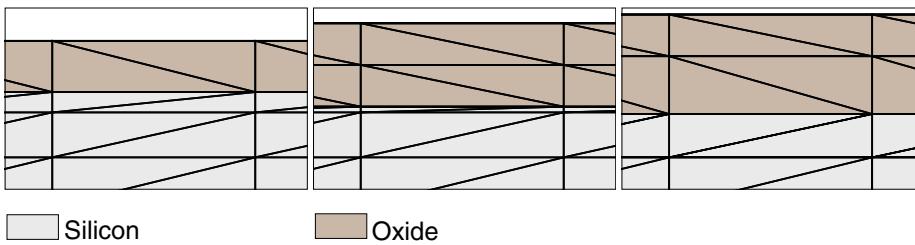


Figure 79 Meshing strategy during thermal oxidation

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# CHAPTER 10 Computing Mechanical Stress

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*This chapter discusses the computation of mechanical stress in Sentaurus Process.*

## Overview

Mechanical stress has an important role in process modeling. It controls the structural integrity of the device, the yield from the process depends on stresses, the mobility of charged carriers is changed by stresses, and leakage currents also are a function of the stress in the system.

On a finer scale, stresses can affect dopant diffusion rates by modifying the band gap. They can affect oxidation rates and, therefore, can alter the shapes of thermally grown oxide layers.

In modern process flows, accurate computation of stress is important. However, there is a continual trend toward designing process flows that produce the right types of stress in the device. With appropriate stresses, device performance can be enhanced significantly.

Stress computation simulations are performed in the following distinct steps:

1. Define the equations for mechanics. The equations used in Sentaurus Process define force equilibrium in the quasistatic regime.
2. Define the boundary conditions for these equations. For the elliptic equations that arise from the equations of force equilibrium, boundary conditions are needed on all boundaries. Sentaurus Process allows Dirichlet or Neumann boundary conditions, provided that certain criteria are met. The minimum criterion is to constrain the structure sufficiently so that it has no rigid body modes.
3. Define material properties. This step defines the relationship between stresses and strains. Some materials may hold stresses for a given strain without relaxing; these are *elastic materials*. Other materials may relax the stresses away; these are *viscous or viscoelastic materials*. Sentaurus Process provides viscoelastic constitutive equations for the computation of mechanical stresses. By setting parameters appropriately, the extreme cases of a purely viscous material and a purely elastic material can be simulated as well. The viscoelastic models used in Sentaurus Process provide a choice between the Maxwell model and the standard linear solid model. The viscosity can depend on the local shear stresses, which make the viscosity a locally varying quantity and can lead to nonlinear mechanical behavior. In addition to elastic and viscoelastic materials, there are materials to model irreversible deformation and temperature-dependent volume change.

## 10: Computing Mechanical Stress

### Material Models

4. Define the mechanisms that drive the stresses. In Sentaurus Process, this is performed through intrinsic stresses, thermal mismatch, material growth, lattice mismatch (silicon germanium), and densification. All these processes are additive in the linear elastic regime. In the nonlinear regime, they must be updated from the available stress history.

Stress is solved in all materials. However, during an inert diffusion, the stress computation can be switched off. Parameters describing material behavior, which will be introduced in this chapter, can be found in the parameter database:

```
<material> Mechanics
```

In the following sections, the constitutive equations are discussed in detail. These tensor equations can be split into two components:

- The *dilatational component*, which corresponds to the trace of the tensor, describes the material behavior in the case of a pure volume change.
- The *deviatoric component* describes an arbitrary deformation but without changing the volume.

For example, the strain tensor can be decomposed as follows:

$$\varepsilon_{ij} = \underbrace{\varepsilon'_{ij}}_{\text{deviatoric}} + \underbrace{\frac{1}{3} \left( \sum_k \varepsilon_{kk} \right) \delta_{ij}}_{\text{dilatational}} \quad (938)$$

This decomposition will be used in subsequent equations to discuss the constitutive equation for the dilatational and deviatoric components independently.

---

## Material Models

Sentaurus Process implements the viscous, viscoelastic, and elastic models in a general manner, where the viscous model and elastic model can be derived from the viscoelastic model. The viscous and viscoelastic models use shear stress-dependent viscosity. The elastic model also has anisotropic elasticity where the elastic coefficients depend on the crystal orientation. The plasticity models describe the material behavior beyond yield, independent of the rate of loading.

## Viscoelastic Materials

The viscoelastic material response is characterized by elastic and viscous components. The combined response depends on how elastic and viscous stresses or strains are coupled. Sentaurus Process provides two commonly used combinations:

- Maxwell model
- Standard linear solid model

### Maxwell Model

The viscoelastic behavior for the Maxwell model is obtained by combining elastic and viscous responses in series. The stress-strain equations are written in terms of dilatational and deviatoric components. The equations for the volumetric component of the stress tensor<sup>1</sup> take the form:

$$\frac{\dot{\sigma}_v}{K} + \frac{\sigma_v}{\eta_v(T, \sigma_s)} = 3\dot{\epsilon}_v$$

$$\sum_k \sigma_{kk} = -3p = 3\sigma_v \quad (939)$$

where  $\eta_v$  is the bulk viscosity. In addition, the relation of the stress and strain tensor to the hydrostatic pressure  $p$  is shown. The bulk modulus  $K$  can be computed from the Poisson ratio (PoissRatio) and Young's modulus (YoungsMod) as:

$$K = \frac{\text{YoungsMod}}{3(1 - 2 \cdot \text{PoissRatio})} \quad (940)$$

The deviatoric component of the stress tensor is described by:

$$\frac{\dot{\sigma}'_{ij}}{G} + \frac{\sigma'_{ij}}{\eta'(T, \sigma_s)} = 2\dot{\epsilon}'_{ij} \quad (941)$$

where  $\eta'$  is the shear viscosity. The shear modulus  $G$  can be computed from the Poisson ratio and Young's modulus as:

$$G = \frac{\text{YoungsMod}}{2(1 + \text{PoissRatio})} \quad (942)$$

---

1. The subscripts of vectors and tensors hold for the Cartesian coordinates x, y, and z.

## 10: Computing Mechanical Stress

### Material Models

By default, the viscoelastic response is applied to the deviatoric components. The linear elastic model is used for the pressure–volume response, that is:

$$\sigma_v = K \sum_k \epsilon_{kk} \quad (943)$$

To apply the viscoelastic response to both the deviatoric components and the volumetric component, use:

```
pdbSet Mechanics NoBulkRelax 0
```

The shear viscosity  $\eta'$  is a function of the shear stress and the temperature  $T$ , where:

$$\eta'(T) = \text{Viscosity0} \cdot \exp\left(-\frac{\text{ViscosityW}}{k_B T}\right) \quad (944)$$

Usually, the value of `ViscosityW` is negative and, therefore, the shear viscosity  $\eta'$  decreases with increasing temperature. The bulk viscosity has a similar Arrhenius expression defined by the parameters `Viscosity0.K` and `ViscosityW.K`. The dependency on the shear stress  $\sigma_s$  is discussed in [Shear Stress–Dependent Viscosity on page 682](#).

## Standard Linear Solid Model

In the standard linear solid model, the material behavior is modeled by combining the elastic response in parallel with the Maxwell model–based viscoelastic response:

$$\sigma_{ij} = \sigma_{ij}^{\text{el}} + \sigma_{ij}^{\text{ve}} \quad (945)$$

where  $\sigma_{ij}^{\text{el}}$  is the elastic stress and  $\sigma_{ij}^{\text{ve}}$  is the viscoelastic stress. The difference compared to the Maxwell model allows the total stress to be nonzero even after the viscoelastic stress has relaxed away:

$$\sigma_{ij}(t \rightarrow \infty) = \sigma_{ij}^{\text{el}} \quad (946)$$

The dilatational and deviatoric components of the elastic and viscoelastic stresses are written in the usual form:

$$\begin{aligned} \sigma_v^{\text{el}} &= 3K_{\text{base}}\epsilon_v \\ \sigma_{ij}^{\text{el}} &= 2G_{\text{base}}\epsilon'_{ij} \\ \frac{\dot{\sigma}_v^{\text{ve}}}{K} + \frac{\sigma_v^{\text{ve}}}{\eta_v(T, \sigma_s^{\text{ve}})} &= 3\dot{\epsilon}_v \\ \frac{\dot{\sigma}_{ij}^{\text{ve}}}{G} + \frac{\sigma_{ij}^{\text{ve}}}{\eta'(T, \sigma_s^{\text{ve}})} &= 2\dot{\epsilon}'_{ij} \end{aligned} \quad (947)$$

where:

- $K_{\text{base}}$  and  $G_{\text{base}}$  are the bulk and shear moduli for the elastic response, respectively.
- $K$  and  $G$  are the bulk and shear moduli for the elastic component of the viscoelastic response, respectively.
- $\eta_v$  and  $\eta'$  are the bulk and shear viscosities, respectively.
- $\varepsilon_v$  and  $\varepsilon'_{ij}$  are the dilatational and the deviatoric components of mechanical strain, respectively.

To enable the standard linear solid model, use:

```
pdbSetSwitch <material> Mechanics ViscoElasticity.Model SLS-Maxwell
```

The default value for the above parameter is `Maxwell` for the Maxwell model.

The elastic response for the standard linear solid model is inactive, by default, so that the material behavior is similar to that of the Maxwell model. The elastic response can be activated by providing nonzero values for the bulk and shear moduli:

```
pdbSetDouble <material> Mechanics BaseBulkModulus <n>
pdbSetDouble <material> Mechanics BaseShearModulus <n>
```

The material parameters for the viscoelastic response are specified in the same way as for the Maxwell model. By default, the dilatational component of viscoelastic stress is assumed to be purely elastic:

$$\sigma_v^{\text{ve}} = 3K\varepsilon_v \quad (948)$$

To activate the viscoelastic response for the dilatational component, use:

```
pdbSet Mechanics NoBulkRelax 0
```

To visualize elastic and viscoelastic responses, this model provides additional output fields. Stresses and strains for the elastic response can be viewed with the `BaseStressEL` and `BaseElasticStrainEL` fields, respectively. Creep strains  $\varepsilon_{ij}^{\text{cr}}$  for the viscoelastic response can be viewed with the `CreepStrainEL` field:

$$\varepsilon_{ij}^{\text{cr}} = \int_0^t \left( \frac{\sigma_v^{\text{ve}}}{2\eta_v} + \frac{\sigma'_{ij}^{\text{ve}}}{2\eta'} \right) dt \quad (949)$$

The solution for viscoelastic stress is time dependent. It also becomes nonlinear when viscosity is a function of viscoelastic shear stress. Therefore, the Newton method is used to solve for stresses. At the end of each Newton iteration, a check is made on whether the convergence criteria have been satisfied. More iterations are performed until all the criteria are satisfied within the specified tolerance or until the maximum number of iterations is reached. For details

about convergence criteria and time-stepping for mechanics, see [Time-Step Control for Mechanics on page 893](#).

## Purely Viscous Materials

Oxide and nitride, by default, are treated as viscoelastic materials. However, the viscosity is a function of temperature (see [Eq. 944](#)). With increasing temperature, the viscosity decreases, that is, the material becomes increasingly more liquid. When the viscosity reaches a very low value, the first term in [Eq. 941](#) can be neglected:

$$\frac{\sigma'_{jk}}{\eta'(T, \sigma_s)} = 2\dot{\epsilon}'_{jk} \Leftrightarrow \sigma'_{jk} = 2\eta'\dot{\epsilon}'_{jk} \quad (950)$$

[Eq. 950](#) describes the deviatoric component of a purely viscous material. The relaxation time  $\tau = \eta'/G$  typically gives a good estimate of the behavior of a viscoelastic material. If  $\tau$  is much greater than the process time, the material is in the elastic regime. The material behaves viscoelastically if  $\tau$  is in the range of the process time. If  $\tau$  is very small, the material is in the viscous regime.

### Shear Stress–Dependent Viscosity

For viscous and viscoelastic materials, the viscosity may depend on the temperature and the shear stress  $\sigma_s$ . The temperature dependency is described by [Eq. 944](#). The dependency on the shear stress is given by:

$$\eta(\sigma_s, T) = \eta(T) \cdot \frac{\sigma_s/\sigma_{\text{crit}}}{\sinh(\sigma_s/\sigma_{\text{crit}})} \quad (951)$$

The shear stress  $\sigma_s$  is computed from the local stress distribution based on the second invariant of the deviatoric component of the stress tensor:

$$\sigma_s = \sqrt{\frac{3}{2} \sum_j \sum_k \sigma'_{jk} \sigma'_{kj}} \quad (952)$$

The viscosity breakdown value  $\sigma_{\text{crit}}$  can be determined by:

$$\sigma_{\text{crit}} = \frac{2k_B T}{v_{\text{crit}}} \quad (953)$$

where:

$$v_{\text{crit}}(T) = V_{\text{crit0}} \cdot \exp\left(-\frac{V_{\text{critW}}}{k_B T}\right) \quad (954)$$

By default, oxide and nitride are treated as viscoelastic materials with shear stress-dependent viscosity. The values for `Vcrit0` and `VcritW` also are set in the parameter database:

```
pdbSetDouble <material> Mechanics Vcrit0
pdbSetDouble <material> Mechanics VcritW
```

## Purely Elastic Materials

If the viscosity in [Eq. 941, p. 679](#) is chosen high enough, the second term on the left can be neglected and the equation reads:

$$\frac{\dot{\sigma}'_{jk}}{G} = 2\dot{\epsilon}'_{jk} \Leftrightarrow \sigma'_{jk} = 2G\epsilon'_{jk} \quad (955)$$

This equation describes the deviatoric component of a purely elastic material. By default, silicon and polycrystalline silicon are treated as purely elastic materials. To achieve this, the viscosity of these materials is set to  $1\times10^{40}$  poise.

**NOTE** *K* and *G* are the primary parameters describing elastic materials, and not Young's modulus and the Poisson ratio. When changing material properties with the `pdb` command, only a change to the primary parameters affects the simulation. To obtain Young's modulus and the Poisson ratio, use the commands [KG2E on page 1035](#) and [KG2nu on page 1036](#), respectively.

**NOTE** When material data is given in terms of Young's modulus and the Poisson ratio, use the commands [Enu2G on page 949](#) and [Enu2K on page 950](#) to convert them to the shear modulus and the bulk modulus, respectively.

## Anisotropic Elastic Materials

The stress and strain relations for anisotropic elastic materials can be described using:

$$\sigma_i = C_{ij}\epsilon_j \quad (956)$$

where  $\sigma_i$  and  $\epsilon_j$  are the components of the engineering stress and strain, respectively, and  $C_{ij}$  is the component of the stiffness matrix. The engineering stress  $\sigma_i$  ( $i=1, \dots, 6$ ) corresponds to the stress-tensor components  $\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}, \sigma_{yz}, \sigma_{xz}$ , and the engineering strain  $\epsilon_j$  ( $j=1, \dots, 6$ ) corresponds to the strain-tensor components  $\epsilon_{xx}, \epsilon_{yy}, \epsilon_{zz}, 2\epsilon_{xy}, 2\epsilon_{yz}, 2\epsilon_{xz}$ .

## 10: Computing Mechanical Stress

### Material Models

**NOTE** The engineering shear-strain components differ from the shear-strain tensor components by a factor of 2.

## Cubic Crystal Anisotropy

The mechanical responses of a crystalline solid vary along various crystal orientations. For a cubic crystal, the axes of reference are chosen to be parallel to the crystal axes. In a coordinate system with axes aligned along the crystal axes, the symmetric stiffness matrix  $C$  has the following nonzero components:  $C_{11} = C_{22} = C_{33}$ ,  $C_{12} = C_{23} = C_{13}$ ,  $C_{44} = C_{55} = C_{66}$ .

All other components are zeros. The anisotropic stress and strain relation is completely defined when three independent modulus parameters  $C_{11}$ ,  $C_{12}$ , and  $C_{44}$  are specified.

The degree of anisotropy for a given material can be measured by the departure from unity of the ratio  $A = 2 C_{44}/(C_{11} - C_{12})$ . The anisotropic model reduces to the isotropic model if the ratio  $A$  is equal to 1. When the simulation coordinate axes do not coincide with the crystal axes, the stiffness matrix  $C$  must be transformed accordingly. For this, note that  $C$  is actually a rank-4 tensor.

By default, the anisotropic elasticity model is switched off. The following command switches on the model:

```
pdbSet Silicon Mechanics Anisotropic 1
```

The values of these three modulus parameters with respect to the cubic crystal axis can be defined using the following commands, which also show the default values for the crystalline silicon:

```
pdbSet Silicon Mechanics C11 16.57E11  
pdbSet Silicon Mechanics C12 6.39E11  
pdbSet Silicon Mechanics C44 7.96E11
```

The unit for these default values is  $\text{dyn/cm}^2$ .

This model depends on the `wafer.orient` and `slice.angle` parameters specified in the `init` command.

## Hexagonal Crystal Anisotropy

The mechanical responses of a crystalline solid vary along various crystal orientations. Hexagonal close-packed crystals contain a plane of isotropy. In a coordinate system with axes aligned along the crystal axes, the symmetric stiffness matrix  $C$  has the following nonzero components:  $C_{11} = C_{22}$ ,  $C_{33}$ ,  $C_{12}$ ,  $C_{13} = C_{23}$ ,  $C_{44} = C_{55}$ ,  $C_{66} = (C_{11} - C_{12})/2$ .

All other components are zeros. The anisotropic stress and strain relation is completely defined when five independent modulus parameters C<sub>11</sub>, C<sub>12</sub>, C<sub>13</sub>, C<sub>33</sub>, and C<sub>44</sub> are specified.

When the simulation coordinate axes do not coincide with the crystal axes, the stiffness matrix  $C$  must be transformed accordingly. The transformation depends on the crystal orientation information specified in the `init` command and the `mater` command.

The values of these five modulus parameters with respect to the crystal axis can be defined using the following commands, which also show the default values for crystalline GaN:

```

pdbSet <material> Mechanics C11 39.0E11
pdbSet <material> Mechanics C12 14.5E11
pdbSet <material> Mechanics C13 10.6E11
pdbSet <material> Mechanics C33 39.8E11
pdbSet <material> Mechanics C44 10.5E11

```

The unit for these default values is dyn/cm<sup>2</sup>.

The hexagonal anisotropic elasticity model is applied to certain wurtzite III–V nitride materials. The following command switches on the model:

```
pdbSet <material> Mechanics Anisotropic 1
```

The material must be set to crystalline with hexagonal lattice type.

## Orthotropic Model

Orthotropic materials have three planes of symmetry. In a coordinate system with axes aligned along the symmetry planes, the symmetric stiffness matrix  $C$  has the following nonzero components:  $C_{11}$ ,  $C_{22}$ ,  $C_{33}$ ,  $C_{44}$ ,  $C_{55}$ ,  $C_{66}$ ,  $C_{12} = C_{21}$ ,  $C_{13} = C_{31}$ ,  $C_{23} = C_{32}$ . The symmetry planes of the model coincide with the simulation coordinate system, and the axes 1, 2, and 3 become axes X, Y, and Z in the simulation coordinate system, respectively.

Orthotropic material properties can be described by specifying nine independent parameters, namely, the Young's moduli in the symmetry planes ( $E_x$ ,  $E_y$ ,  $E_z$ ), the directional shear moduli ( $G_{xy}$ ,  $G_{xz}$ ,  $G_{yz}$ ), and the directional Poisson ratios ( $\nu_{xy}$ ,  $\nu_{xz}$ ,  $\nu_{yz}$ ). The other directional Poisson ratios are calculated from:

$$\frac{\nu_{ij}}{E_i} = \frac{\nu_{ji}}{E_j} \quad (957)$$

where  $i, j = x, y, z$ .

## 10: Computing Mechanical Stress

### Material Models

The stiffness matrix components are calculated from the specified material properties as:

$$\begin{aligned} C_{11} &= E_x(1 - \nu_{yz}\nu_{zy}) \times \gamma \\ C_{22} &= E_y(1 - \nu_{xz}\nu_{zx}) \times \gamma \\ C_{33} &= E_z(1 - \nu_{xy}\nu_{yx}) \times \gamma \\ C_{12} &= C_{21} = E_x(\nu_{yx} + \nu_{yz}\nu_{zx}) \times \gamma \\ C_{13} &= C_{31} = E_z(\nu_{xz} + \nu_{xy}\nu_{yz}) \times \gamma \\ C_{23} &= C_{32} = E_y(\nu_{zy} + \nu_{zx}\nu_{xy}) \times \gamma \\ \gamma &= (1 - \nu_{xy}\nu_{yx} - \nu_{yz}\nu_{zy} - \nu_{xz}\nu_{zx} - 2(\nu_{yx}\nu_{xz}\nu_{zy}))^{-1} \end{aligned} \quad (958)$$

$$\begin{aligned} C_{44} &= G_{yz} \\ C_{55} &= G_{xz} \\ C_{66} &= G_{xy} \end{aligned} \quad (959)$$

By default, the orthotropic model is switched off. It is switched on using the command:

```
pdbSet <material> Mechanics Orthotropic 1
```

The material properties can be specified by the command:

```
pdbSetDouble <material> Mechanics <material_parameter> <n>
```

specifically:

```
pdbSetDouble <material> Mechanics YoungsModulusX <n>
pdbSetDouble <material> Mechanics YoungsModulusY <n>
pdbSetDouble <material> Mechanics YoungsModulusZ <n>
pdbSetDouble <material> Mechanics PoissonRatioXY <n>
pdbSetDouble <material> Mechanics PoissonRatioXZ <n>
pdbSetDouble <material> Mechanics PoissonRatioYZ <n>
pdbSetDouble <material> Mechanics ShearModulusXY <n>
pdbSetDouble <material> Mechanics ShearModulusXZ <n>
pdbSetDouble <material> Mechanics ShearModulusYZ <n>
```

The units for Young's modulus and the shear modulus are  $\text{dyn/cm}^2$ .

Orthotropic thermal expansion also is considered in this material model, and different coefficients of thermal expansion can be specified along the three symmetry planes:

```
pdbSetDouble <material> Mechanics ThExpCoeffX <n>
pdbSetDouble <material> Mechanics ThExpCoeffY <n>
pdbSetDouble <material> Mechanics ThExpCoeffZ <n>
```

Temperature-dependent material properties can be specified for all the material parameters specified above. The variation of a property  $\xi$  can be specified as:

$$\xi(T) = \xi_{\text{ref}} + \xi(T - T_{\text{ref}}) \quad (960)$$

where the reference value is the material parameter value specified in the command file.

The values can be specified as:

```
pdbSet <material> Mechanics <material parameter>Rate <n>
```

For example:

```
pdbSetDouble FR4 Mechanics ThExpCoeffXRate 0
```

These orthotropic parameter entries exist for silicon, and the shorthand `pdbSet` command can be used. The default values are set to replicate isotropic elastic behavior.

**NOTE** The older parameters using the 1, 2, 3 indices are deprecated and are replaced with the new parameters using the X, Y, Z indices.

**NOTE** Anisotropic elastic models and plastic models must not be switched on simultaneously for the same material.

## Plastic Materials

Materials such as metals show linear elastic behavior at lower stresses but undergo permanent deformation at higher stresses. At low temperatures, permanent deformation in these materials is not sensitive to the rate of loading. Such material behavior is defined as plastic or elastic-plastic.

To switch on the plastic material model, use the command:

```
pdbSet <material> Mechanics IsPlastic <n>
```

### Incremental Plasticity

Plastic material behavior under nonmonotonic loading is modeled using incremental formulation.

## 10: Computing Mechanical Stress

### Material Models

Incremental plasticity uses the von Mises yield criterion with associative flow and bilinear hardening. The von Mises yield criterion for isotropic solid materials takes the form:

$$F(\sigma'_{ij}, q_{ij}, \alpha) = \sqrt{(\sigma'_{ij} - q_{ij})(\sigma'_{ij} - q_{ij})} - Y(\alpha) = 0 \quad (961)$$

where:

- $q_{ij}$  is the back stress.
- $\alpha$  is an isotropic hardening variable.
- $Y(\alpha)$  is a function describing the change of yield surface with progressive yielding. This function can be set to linear or exponential with:

```
pdbSetSwitch <material> Mechanics Incremental.Plasticity.Yield.Model
    <Linear | Exponential>
```

The linear relation takes the form  $Y(\alpha) = \sqrt{\frac{2}{3}}(\sigma_y + H_{iso}\alpha)$  where  $\sigma_y$  is the yield stress in uniaxial tension, and  $H_{iso}$  is the isotropic hardening modulus.  $\sigma_y$  and  $H_{iso}$  can be set respectively using the commands:

```
pdbSetDouble <material> Mechanics Incremental.Plasticity.SigmaY <n>
    pdbSetDouble <material> Mechanics Incremental.Plasticity.Hiso <n>
```

The exponential relation takes the form  $Y(\alpha) = \sqrt{\frac{2}{3}}(\sigma_y + R_{iso}(1 - \exp(-b_{iso}\alpha)))$  where  $R_{iso}$  and  $b_{iso}$  are parameters for nonlinear (exponential) isotropic hardening. To set these parameters, use the commands:

```
pdbSetDouble <material> Mechanics Incremental.Plasticity.Riso <n>
    pdbSetDouble <material> Mechanics Incremental.Plasticity.Biso <n>
```

Under a small strain assumption, the strains (and strain rates) are decomposed additively:

$$\dot{\epsilon}_{ij} = \dot{\epsilon}_{ij}^e + \dot{\epsilon}_{ij}^p \quad (962)$$

where  $\dot{\epsilon}_{ij}^e$  are the elastic strains, and  $\dot{\epsilon}_{ij}^p$  are the plastic strains.

For incremental plasticity, the plastic strains are determined by the plastic flow rule:

$$\dot{\epsilon}_{ij}^p = \dot{\gamma} \frac{\partial Q}{\partial \sigma_{ij}} \quad (963)$$

where  $\dot{\gamma} \geq 0$  is the slip rate, and  $Q$  is the plastic potential. Plastic flow is assumed to be volume preserving, so that plastic strain is purely deviatoric:

$$\epsilon_{ij}^p \delta_{ij} = 0 \Rightarrow \epsilon_{ij}^p = \epsilon_{ij}^p \quad (964)$$

For associative plastic flow, the plastic potential  $Q$  is set equal to the yield function  $F$ . The evolution of the isotropic hardening variable and the back-stress variable is given by:

$$\dot{\alpha} = \dot{e}^p = \sqrt{\frac{2}{3}}\dot{\gamma}$$

$$\dot{q}_{ij} = \frac{2}{3}\dot{\gamma} \left( H_{\text{kin}} \frac{(\sigma'_{ij} - q_{ij})}{\sqrt{(\sigma'_{kl} - q_{kl})(\sigma'_{kl} - q_{kl})}} - \sqrt{\frac{3}{2}}H_{\text{NLkin}}q_{ij} \right) \quad (965)$$

where  $H_{\text{kin}}$  is the linear kinematic hardening modulus,  $H_{\text{NLkin}}$  is the parameter for nonlinear kinematic hardening, and  $\dot{e}^p$  is the equivalent plastic strain rate. The Einstein summation convention is used to define the tensor product in this equation.

To set the kinematic hardening parameters, use the commands:

```
pdbSetDouble <material> Mechanics Incremental.Plasticity.Hkin <n>
pdbSetDouble <material> Mechanics Incremental.Plasticity.HNLkin <n>
```

For linear isotropic hardening, the hardening modulus is interpreted as the slope of the stress versus the plastic strain curve (as obtained from uniaxial tension test)  $H_{\text{iso}} = \frac{d\sigma}{d\epsilon^p}$ .

It differs from the elastic-plastic tangent modulus, which is defined as the slope of the stress versus total strain curve  $E^{ep} = \frac{d\sigma}{d\epsilon}$ .

To switch on the incremental plasticity model, use:

```
pdbSet <material> Mechanics Plasticity.Model Incremental
```

The rate equations are discretized using the backward Euler scheme and then are solved using a radial return mapping algorithm (see [1] for more details).

The nonlinear nature of the plasticity model requires Newton iterations to achieve the equilibrium state for each loading step. At the end of each iteration, a check on the satisfaction of convergence criteria is made. More Newton iterations are performed until all the convergence criteria are satisfied within the specified tolerance or until the maximum number of iterations is reached. See [Time-Step Control for Mechanics on page 893](#) for details on convergence criteria and time-stepping for mechanics.

**NOTE** To define the plastic model, use nonzero values for the isotropic or the kinematic hardening modulus along with yield stress. In the absence of hardening, the numeric simulation of plastic deformation may become unstable.

**NOTE** The PDB parameters Hardening.Modulus.Isotropic, FirstYield, and Hardening.Modulus.Kinematic are deprecated and are replaced by Incremental.Plasticity.Hiso, Incremental.Plasticity.SigmaY, and Incremental.Plasticity.Hkin, respectively.

---

## Mole Fraction–Dependent Mechanical Properties of Compound Materials

The mechanical properties of compound materials change with the ratio of substance concentration, that is, mole fraction. For general information about alloys, mole fraction computation, and parameter interpolation, see [Alloy Materials and Parameter Interpolation on page 25](#).

In mechanics, mole fraction dependency is used by default and is applied to:

- The bulk modulus and the shear modulus for isotropic materials.
- $C_{11}$ ,  $C_{12}$ , and  $C_{44}$  for cubic anisotropic elastic materials.
- $C_{11}$ ,  $C_{12}$ ,  $C_{13}$ ,  $C_{33}$ , and  $C_{44}$  for hexagonal anisotropic elastic materials.
- The coefficient of thermal expansion.

The alloy mechanics parameters are interpolated based on the mole fraction and the parameters defined on the base materials. Base materials are non-alloy materials that form the alloy. For example, the elastic constant  $C_{11}$  of the ternary alloy AlGaN is interpolated from the elastic constant  $C_{11}$  of its base materials AlN and GaN. For the binary compound SiGe, the elastic constants are interpolated from the parameters defined on Si and Ge.

The mole fraction dependency for the above-listed mechanical properties can be defined separately. By default, a linear interpolation is used. If the parameter is defined for the compound material, the given parameter value is used.

Mole fraction dependency can be switched off with:

```
pdbSet Mechanics Parameter.Interpolation 0
```

---

## Temperature–Dependent Mechanical Properties

The mechanical properties of materials are different at high temperature from those at room temperature. The elastic modulus of typical materials decreases as temperature rises. Some materials show nonnegligible changes of mechanical properties at different temperatures.

The temperature dependency and mole fraction dependency are handled under the same PDB switch. The temperature dependency can be applied to:

- The bulk modulus and the shear modulus for isotropic materials.
- $C_{11}$ ,  $C_{12}$ , and  $C_{44}$  for cubic anisotropic elastic materials.
- $C_{11}$ ,  $C_{12}$ ,  $C_{13}$ ,  $C_{33}$ , and  $C_{44}$  for hexagonal anisotropic elastic materials.
- The coefficient of thermal expansion for isotropic, cubic anisotropic, and hexagonal anisotropic elastic materials.

Table 82 Temperature-dependent mechanical parameters

Material model	PDB parameters
Isotropic elasticity	BulkModulus, ShearModulus, ThExpCoeff
Cubic anisotropic elasticity	$C_{11}$ , $C_{12}$ , $C_{44}$ , ThExpCoeff
Hexagonal anisotropic elasticity	$C_{11}$ , $C_{12}$ , $C_{13}$ , $C_{33}$ , $C_{44}$ , ThExpCoeff1, ThExpCoeff2, ThExpCoeff3
Other	Refer to the corresponding sections for related parameters and syntax

The temperature dependency for the above-listed mechanical properties can be defined separately. The available options are:

- The linear dependency is defined with the parameter `<parameter>.T1`, for example:  

```
pdbSet <material> Mechanics BulkModulus.T1 <n>
```
- Then, the parameter is calculated using  $P(T) = P + P.T1(T - 26.85)$ , where the unit of temperature is degree Celsius.
- The piecewise linear dependency can be specified with:  

```
pdbSetDoubleArray SiliconGermanium Mechanics ShearModulus.TTable
{<T1> <v1> ... <Tn> <vn>}
```

The unit of temperature is degree Celsius. The linear dependency defined by `<parameter>.T1` is ignored.

The temperature dependency can be switched off with:

```
pdbSet Mechanics Parameter.Interpolation 0
```

**NOTE** Do not mix new syntax with old syntax (see [Plane Stress Analysis on page 692](#)). Some of the old syntax might exist in the Advanced Calibration script.

## 10: Computing Mechanical Stress

### Plane Stress Analysis

---

## Plane Stress Analysis

In 2D problems, the elastic models implemented in Sentaurus Process follow the plane strain formulation by default. Under the plane strain assumption:

$$\varepsilon_{zz} = 0; \sigma_{zz} \neq 0 \quad (966)$$

While this is good for structures where the strain in the third direction is very small compared to the cross section, it would give inaccurate results for thin structures. Thin plate-like structures where one dimension is very small compared to the other two can be modeled under the plane stress assumption:

$$\varepsilon_{zz} \neq 0; \sigma_{zz} = 0 \quad (967)$$

The strain  $\varepsilon_{zz}$  is obtained as a function of other strains, for example, for purely elastic structures:

$$\varepsilon_{zz} = -\nu(\varepsilon_{xx} + \varepsilon_{yy}) \quad (968)$$

The plane stress model can be switched on for a particular region using:

```
pdbSetBoolean <material> Mechanics PlaneStress 1
```

**NOTE** You must switch on the plane stress model in all regions. Combining plane stress and plane strain formulations within a structure by switching on plane stress in only a few regions is *not* advisable.

---

## Equations: Global Equilibrium Condition

The equations for mechanics in Sentaurus Process are the quasistatic equations of force equilibrium.

The strain rate tensor is related to the symmetric component of the velocity gradient and is given by:

$$\dot{\varepsilon}_{jk} = \frac{1}{2}\left(\frac{\partial v_j}{\partial x_k} + \frac{\partial v_k}{\partial x_j}\right) \quad (969)$$

Strain is then related to stresses through any of the models defined in [Material Models on page 678](#). For all models, the global equilibrium condition is given by:

$$\sum_k \frac{\partial \sigma_{jk}(\mathbf{v})}{\partial x_k} = 0 \quad (970)$$

The above equations are solved using the finite-element method. The solution is a vector representing the velocity components at each node. These velocities are used to compute the strain and stresses. The stresses and the boundary conditions determine the mechanical state of the system.

**NOTE** Stress and strain are derivatives of velocity. They are, therefore, computed at one order of accuracy lower than the solution variable. This also means that they are discontinuous across the elements. When visualized, the stress values may appear poorly converged even if the linear solver has converged.

In addition, the quasistatic mechanics equations are elliptic in nature and, therefore, are prone to high levels of shape dependency. This is most frequently seen at gate corners during polysilicon reoxidation steps or at the corners of the STI trench during liner oxidation. These equations also exhibit a high sensitivity to the mesh modification algorithms at these corners.

**NOTE** At sharp corners, the mechanics equations have a singularity. Therefore, it is not possible to discretize at a corner correctly using regular types of element.

---

## Boundary Conditions

Equations for stress equilibrium require boundary conditions to define the system completely.

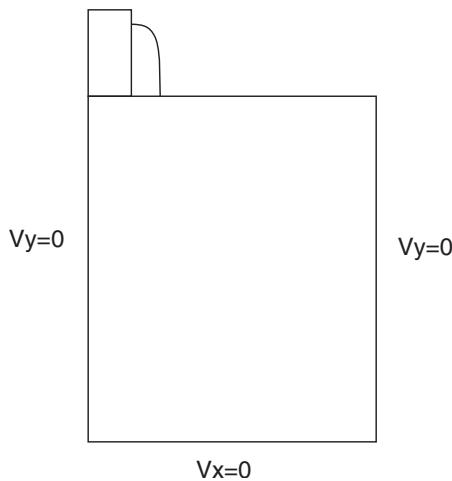


Figure 80 Default mechanics boundary conditions in the unified coordinate system

The default boundary conditions are zero velocities in the direction perpendicular to the boundary planes. Since velocities are set to fixed values along the boundaries, these boundary

## 10: Computing Mechanical Stress

### Boundary Conditions

conditions are referred to as Dirichlet boundary conditions in directions perpendicular to boundary planes. The HomNeumann boundary condition is used when the plane must be free.

Sentaurus Process provides a general way to reset the default boundary conditions and specify boundary conditions for stress analysis using the `stressdata` command:

```
stressdata bc.location= Left | Right | Front | Back | Bottom  
bc.value= {dx=<n> | dy=<n> | dz=<n>}
```

The arguments `dx`, `dy`, and `dz` specify the displacement rates (default unit: cm/s).

The displacement rates are applied to the area defined by `bc.location`, where `Left`, `Right`, `Front`, `Back`, and `Bottom` refer to the outer boundary surfaces of the simulation domain. At least at one node, the displacement along any coordinate system direction must be fixed to remove the rigid body motion.

**NOTE** Any boundary condition defined with the `stressdata` command invalidates the default boundary conditions. If no boundary condition is defined, free boundary condition is applied by default.

Dirichlet boundary conditions are imposed using the penalty method, by default. To adjust the penalty factor, use the command:

```
pdbSet Mechanics Boundary.Penalty.Factor <n>
```

The default penalty factor is `1.0e12`. The larger this factor, the more accurate the enforcement of Dirichlet boundary conditions. However, using an extremely large penalty factor could lead to an ill-conditioned matrix and, therefore, could slow down the linear equation solver.

Alternatively, you can use the matrix reduction method to impose Dirichlet boundary conditions. To choose the penalty method or matrix reduction method, use the command:

```
pdbSet Mechanics Boundary.Method.Type <model>
```

where `<model>` is `Penalty` or `MatrixReduction`.

**NOTE** To ensure the structure is bounded by a perfect rectangle, the displacements computed by these general boundary conditions are not applied to the structure. However, they evaluate the stresses correctly. This assumption is consistent with the small deformation assumption within each mechanics time step.

---

## Example: Applying Boundary Conditions

This 2D example simulates silicon covered with oxide, with the right side free to move:

```
line x loc= -0.02 tag= e spacing= 0.005
line x loc= 0      tag= a spacing= 0.005
line x loc= 0.2    tag= b spacing= 0.05

line y loc= 0 tag= c spacing= 0.05
line y loc= 2 tag= d spacing= 0.05

region silicon xlo= a xhi= b ylo= c yhi= d
region oxide xlo= e xhi= a ylo= c yhi= d

init !DelayFullD

pdbSetDouble Mechanics RefThExpCoeff 0
stressdata bc.location= Bottom bc.value= { dx=0 }
stressdata bc.location= Left bc.value= { dy=0 }

pdbSet Oxide Mechanics Viscosity0 1e40
pdbSet Oxide Mechanics ViscosityW 0

temp_ramp name= tr1 temperature= 600 ramprate= 30<K/min> time= 10<min>
diffuse temp.ramp= tr1

struct tdr= rampup
diffuse time= 10 temperature= 900 wet
struct tdr= postout
```

## Deprecated Syntax

You can select various boundary conditions using:

```
pdbSet Mechanics <side> BoundaryCondition <model>
```

where:

- <side> is Left, Right, Front, or Back.
- <model> is HomNeumann or Dirichlet.

## 10: Computing Mechanical Stress

### Boundary Conditions

The HomNeumann boundary condition is used when the plane must be free and implies a zero normal stress (shown in [Figure 81](#)).

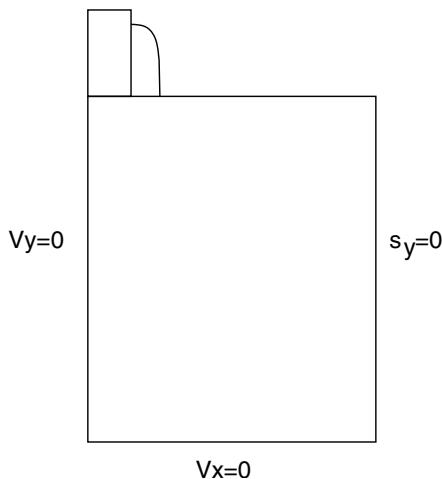


Figure 81 HomNeumann boundary condition on right boundary plane

For example, if you want to set the right plane to be free, use the command:

```
pdbSet Mechanics Right BoundaryCondition HomNeumann
```

**NOTE** Any boundary condition or loading condition defined with the `stressdata` command invalidates all boundary conditions defined with `pdbSet Mechanics <side> ...`, including the default ones.

---

## Pressure Boundary Condition

The pressure boundary condition is used to apply uniform pressure on the exterior boundary. The direction of the loading depends on the normal of the exterior surface. To apply the pressure boundary condition, use the `stressdata` command, for example:

```
stressdata bc.location= Left | Right | Front | Back | Bottom  
bc.value= {pressure=<n>}
```

---

## Periodic Boundary Condition

The periodic boundary condition is used for structures with a periodically repeating pattern. This condition is used on periodic structures with assigned master and slave boundaries. The slave boundary has the same deformation profile as the master boundary.

In [Figure 82](#), the left and right boundaries are bound together by the periodic boundary condition.

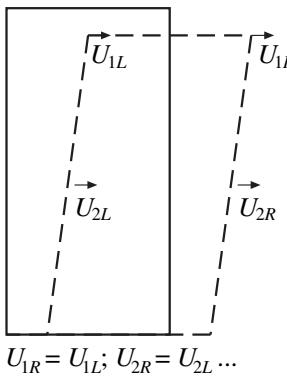


Figure 82 Periodic boundary condition

To apply the periodic boundary condition to the outer bounding surfaces, use the command:

```
pdbSet Mechanics <Left | Right | Front | Back> Periodic 1
```

If this command is specified on a sidewall, the opposite sidewall is defined automatically as a periodic boundary. Conflicts of boundary condition definitions are checked on all sidewalls. For example, to apply a periodic boundary condition on the left and right sidewalls, use one of the following commands:

```
pdbSet Mechanics Left Periodic 1
pdbSet Mechanics Right Periodic 1
```

Both the periodic and coupling boundary conditions are implemented using the penalty method. To adjust the penalty factor, use the command:

```
pdbSet Mechanics Constraint.Penalty.Factor <n>
```

The default penalty factor is  $1.0 \times 10^{13}$ . The larger this factor, the more accurately the periodic or coupling boundary conditions will be enforced. Using an extremely large penalty factor could lead to an ill-conditioned matrix and, therefore, slow down or even fail the linear equation solver.

**NOTE** If you choose to apply periodic boundary conditions, all other boundary conditions defined through the old `pdbSet` method will be ignored and must be redefined using the `stressdata` command.

## Time-Step Control

It may be necessary to use time step control when viscous or viscoelastic materials are present in the structure. Usually, when other dopants also are present, the time steps will be sufficiently limited by the diffusion solver. If dopants are not present or for materials with a low viscosity, the time step control for the Maxwell model can be switched on with:

```
pdbSet Mechanics Visc.Step.Control 1
```

Time-stepping can be controlled with both the displacement increment and the relative relaxation time. To switch on these two options, use the following commands:

```
pdbSet Mechanics Visc.Step Limit.Disp 1  
pdbSet Mechanics Visc.Step Limit.ScaleT 1
```

To see other control parameters, launch the PDB Browser, and see the section **Mechanics > Visc.Step**.

For the standard linear solid model for viscoelasticity, time-step control is activated automatically (see [Time-Step Control for Mechanics on page 893](#)).

---

## Stress-Causing Mechanisms

Every mechanical system needs a set of stress-driving mechanisms to reach a stressed state. The stress-inducing mechanisms in Sentaurus Process are described here.

---

## Growth of Material

During the oxidation process, volume is *produced*. Consuming silicon of volume 1 during thermal oxidation produces oxide of volume 2.25. This process introduces velocities at a growing interface: A velocity vector pointing into the silicon describes the progress of the oxidation front, and a velocity vector pointing into the oxide accounts for the volume expansion as described above. The latter is responsible for the generation of mechanical stresses and, therefore, is used as a boundary condition for the mechanical problem.

---

## Densification

A typical densification process uses thermal heating to increase the density of a porous material. As the material density increases, its volume shrinks and the volume shrinkage generates stresses.

The densification-induced stress computation is switched on using the `density.increase` parameter in the `diffuse` command or the `temp_ramp` command, such as:

```
diffuse temperature= 1000<C> time= 30<min> \
    density.increase= {<regionName>=<n> | <material>=<n>}

temp_ramp name= dens time= 1 temperature= 1000 density.increase= {oxide=0.02}
diffuse temp.ramp= dens
```

The total amount of density increase can be specified per material or per region for a given `diffuse` (or `temp_ramp`) step as shown above. A proportional amount of density increase is applied during each time step of the densification process.

The densification operation can be performed for all existing materials, as well as new materials defined using the `mater` command:

```
mater add name= TEOS new.like= oxide
diffuse time= 1 temperature= 1000 density.increase= {TEOS= 0.03}
```

For densification processes involving large amounts of volume shrinkage, the material boundaries and meshes can be updated using the following settings:

```
pdbSet Grid Inert.Modify.Mesh 1
pdbSetDouble TEOS Grid MinimumVelocity 0
```

For a complete densification process that has distinguished density changes, multiple `diffuse` steps can be used with different density increases for each segment of the process.

## Selectively Switching Off Grid Movement

The parameter `MinimumVelocity` can be used to selectively switch off point or interface movement. This can be useful, for example, when a mechanics simulation computes a small amount of boundary movement that is either unwanted or could cause element quality to suffer in the vicinity, and the approximation of no movement is acceptable. In general, the command is:

```
pdbSet <material> Grid MinimumVelocity <speed>
```

## 10: Computing Mechanical Stress

### Stress-Causing Mechanisms

If `<material>` is a bulk material (no underscore), the parameter applies to bulk points. If the speed of the bulk points is less than `<speed>` (in cm/s), Sentaurus Process truncates the speed to zero. This truncation is applied to material `Silicon` by default.

On the other hand, if `<material>` is an interface material (with an underscore, such as `PolySilicon_Silicon`), the parameter only applies to points on that interface. This truncation is applied to material `Silicon` by default.

**NOTE** The moving mesh operations can become unstable for values of `MinimumVelocity` that are neither very large nor zero. Very large values stop all motion, and 0 allows all motion.

---

## Thermal Mismatch

Temperature changes during the process described by the `temp_ramp` command or the keyword `ramprate` in the `diffuse` command lead to stress in the structure caused by the different coefficients of thermal expansion of the relevant materials.

When necessary, the stress computation can be switched off using the `stress.relax` flag:

```
diffuse temperature= 1000<C> time= 30<min> !stress.relax
```

**NOTE** If viscous or viscoelastic materials are present in the structure, the stress distribution may change even without a change in the temperature due to viscoelastic relaxation.

By default, stresses are computed during inert annealing for 2D simulations. To apply `!stress.relax` to all inert annealing steps, use the command:

```
pdbSet Compute NoStressRelax 1
```

To apply `stress.relax` to all inert annealing steps in 3D simulations, use the command:

```
pdbSet Diffuse 3DStressRelax 1
```

The coefficient of thermal expansion for certain materials can be found in the parameter database as follows:

```
pdbGet <material> Mechanics ThExpCoeff
```

Thermal expansion only affects the dilatational component of the constitutive equation. For isotropic elasticity, a small temperature change leads to a change in the dilatational stress component according to:

$$\Delta\sigma_{kk} = -3K\alpha_{rel,kk}\Delta T \quad (971)$$

where  $K$  is the bulk modulus at the current temperature. The change in the temperature is described by  $\Delta T$  and  $\alpha_{\text{rel}} = \alpha_{\text{mat}} - \alpha_{\text{subs}}$  is the relative coefficient of thermal expansion of a certain material with respect to the coefficient of thermal expansion of the substrate. The integration of thermal mismatch strain uses the midpoint rule. For anisotropic elasticity, the general tensor expression is used.

For hexagonal anisotropic materials, the coefficient of thermal expansion tensor has a symmetry plane and can be defined with:

```
pdbSet <material> Mechanics ThExpCoeff1 <n>
pdbSet <material> Mechanics ThExpCoeff2 <n>
pdbSet <material> Mechanics ThExpCoeff3 <n>
```

The first two coefficients of thermal expansion must be equal for hexagonal anisotropic materials.

In certain examples, like bending, you may want to use absolute coefficients of thermal expansion instead of relative coefficients of thermal expansion. This can be achieved by setting the parameter `RefThExpCoeff` as follows:

```
pdbSetDouble Mechanics RefThExpCoeff 0.
```

All coefficients of thermal expansion are computed with respect to the substrate. This reference value is changed by setting a certain region as the substrate and resetting the coefficient of thermal expansion. A region can be tagged as the substrate in different ways:

- Use the `substrate` argument when defining regions with the `region` command before the `init` command.
- If a saved structure is being loaded into Sentaurus Process, a region is tagged as the substrate with the command:

```
region name=<c> substrate
```

The reference coefficient of thermal expansion can be directly set with:

```
pdbSetDouble Mechanics RefThExpCoeff <n>
```

This command overwrites the reference coefficient of thermal expansion setting from the substrate.

When doped deposition is used for epitaxial growth of SiGe at constant temperature, no thermal mismatch stress is introduced to the epitaxial layer with the model given by [Eq. 971](#). To account for the thermal mismatch effect in the epitaxially grown materials, use the command:

```
pdbSet Mechanics Compound.ThExpCoeff 1
```

## 10: Computing Mechanical Stress

### Stress-Causing Mechanisms

**NOTE** Unlike the model given by Eq. 971, this model calculates the thermal mismatch stress in SiGe at the current temperature  $T$  without integration over the historical temperature ramps. Specifically, the thermal mismatch strain in SiGe is evaluated as  $\alpha_{\text{rel}} \cdot (T - T_0)$ , where  $T_0$  is the room temperature (300 K) and  $\alpha_{\text{rel}}$  is evaluated at the middle of the current temperature step.

---

## Lattice Mismatch

The presence of impurities, such as germanium and carbon, can change the lattice parameters of crystalline silicon. This effect has been exploited in two ways technologically:

- Introducing an impurity during epitaxy to form a strained layer.
- Growing a substrate (typically, a very thick layer grown on a standard substrate) to produce a customized lattice constant.

However, most technological applications are based on the first use, for example, when SiGe source/drain pockets are grown on silicon substrates. For strained SiGe epitaxy, Sentaurus Process automatically computes and applies the strain, and no user input is necessary.

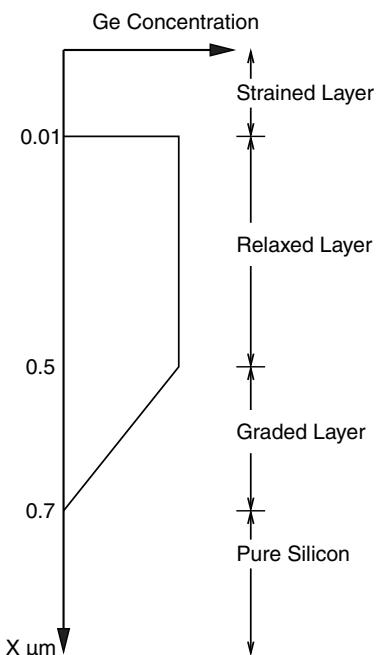


Figure 83 Simple SiGe wafer for customizing the lattice spacing

For customized lattice-spacing substrates or other material systems, more setup is required. This section explains the theory and implementation of this model and gives an example. [Figure 83 on page 702](#) shows a simple SiGe wafer.

There are four main regions of the manufactured substrate. The silicon region has the graded buffer layer where the Ge concentration increases linearly from zero to the required concentration. The manufacturing process of this layer is designed such that all the dislocations are forced energetically to nucleate here, and the wafer is completely relaxed. The relaxed layer that is grown on top of the graded layer has no dislocations and no strain. The lattice spacing of this layer is determined by the Ge mole fraction. The lattice spacing of this layer controls the strains obtained in the top strained layer. The top strained layer is grown depending on the kind of strain required. If this layer is to be in a tensile state, the Ge concentration here must be less than that of the relaxed layer. In the case of a compressive state, the Ge concentration must be greater than that of the relaxed layer. This layer has a thermodynamic limit on its thickness since the strain energy it contains should be less than the dislocation nucleation energy. The strain energy is directly proportional to the volume that is under the strain. The strain profile of germanium in silicon is given approximately by:

$$\epsilon = 0.0425x \quad (972)$$

where  $x$  is the Ge mole fraction calculated as the germanium concentration divided by the silicon lattice density.

In the relaxed region, Sentaurus Process modifies the lattice spacing. This results in no stresses due to the presence of germanium. In the strained region, the lattice spacing is fixed by the lattice spacing in the relaxed region. Now, using the Ge mole fraction in the strained region, the effective unstrained lattice spacing is computed, and the stresses are based on the difference of the effective lattice constant and the lattice constant of the relaxed region.

For example, assume the strained layer has no Ge: The effective lattice constant is that of silicon given by  $L_{Si}$ . The lattice constant of the relaxed SiGe component is, for example,  $L_{SiGe}$ . The strain in the strained region is:

$$\epsilon = \frac{L_{SiGe} - L_{Si}}{L_{Si}} \quad (973)$$

The strain computed using [Eq. 973](#) is applied as a normal strain in the x-, y-, and z-directions.

## Using the Lattice Mismatch Model

For the most common case of SiGe layers grown on silicon substrates, the model is switched on by default, and strain is computed and updated as necessary. For simulating other alloy material systems, a few settings are required to instruct Sentaurus Process how the lattice mismatch strain should be computed.

## 10: Computing Mechanical Stress

### Stress-Causing Mechanisms

If the substrate is not silicon or it is not the bottommost region in the substrate (that is, the largest x-coordinate), you must identify the substrate region in the wafer. Use the `region` command and include the keyword `substrate` for the appropriate region. If there is no substrate defined in the loaded structure, use the following command to tag a region as a substrate:

```
region name=<c> substrate
```

Regions isolated from the substrate by nonsubstrate materials must be tagged as substrate to account for the lattice mismatch effect. The mesh must be up-to-date with the region to be tagged as substrate.

For systems other than SiGe, there are two sources for lattice mismatch strain:

1. For alloy materials, the lattice mismatch strain is computed based on the difference of the local relaxed lattice constant due to varying mole fraction and the reference effective lattice constant. This model applies to both the cubic lattice system and the hexagonal lattice system. For the hexagonal lattice system, the lattice constant in the symmetry plane is used. The lattice constant of the base materials must be defined. The material SiGe is set to be a compound by default, and the strain profile definition is ignored. For more information about compound and alloy materials, see [Diffusion in III-V Compounds on page 251](#).
2. For other impurities that have no effect on the alloy mole fraction, Sentaurus Process must know the strain profile of the field in the substrate. The `strain_profile` command is used to specify this. The strain is specified as a piecewise linear function of the mole fraction. For example, for ImpurityA in silicon, it is:

```
strain_profile Silicon species=ImpurityA strain= {0 0.0425} ratio= {0 1}
```

or:

```
pdbSetDoubleArray Silicon ImpurityA Conc.Strain {0 0 1 0.0425}
```

**NOTE** To revert to the old model to treat SiGe as Si with Ge impurity, and to define the nonlinear strain profile for Ge, use the command:

```
pdbSet Mechanics Lattice.Constant.Mismatch 0
```

The lattice mismatch model for defined alloy materials is switched on by default.

Next, for customized lattice-spacing substrates, the substrate must be given an impurity profile. The profile can be specified with the `profile` command as a piecewise linear function of the x-coordinate:

```
profile region=<c> name=<c> \
concentration= {1e10 1e10 2e22 2e22 1e10 1e10} \
xcoord= {0 0.01 0.011 0.5 0.7 10} linear
```

The location of the top of the relaxed region must be specified in Sentaurus Process. Generally, this should not be at the top of the relaxed layer (see [Figure 83 on page 702](#)) because germanium diffusion during any anneal step can cause unrealistic stress values to appear in this area. The best location for the top of the relaxed region is approximately two-thirds of the relaxed layer thickness from the top of the relaxed layer. In this example, it is approximately 0.35  $\mu\text{m}$ . This reference position can be set with the command:

```
pdbSetDouble Silicon Mechanics TopRelaxedNodeCoord 0.35e-4
```

**NOTE** In most cases, when the simulation does not require any SiGe substrate (for example, when SiGe source/drain pockets are grown on silicon substrates), this parameter is not needed. The reference lattice spacing is the one of the substrate. Sentaurus Process detects automatically the adjacent silicon-like regions and applies to them the lattice mismatch model. For this reason, the value of this parameter defaults to the bottom coordinate of the structure.

The lattice mismatch strain is defined with respect to the lattice constant at the reference position by default. To switch to the lattice constant at the current position, use the command:

```
pdbSetSwitch Mechanics Lattice.Mismatch.Strain LCC
```

The default model is LCR. The lattice mismatch strain for the LCR model is calculated as  $(LC_{\text{ref}} - LC_{\text{relaxed}})/LC_{\text{ref}}$ , while for the LCC model, it is  $(LC_{\text{ref}} - LC_{\text{relaxed}})/LC_{\text{relaxed}}$ , where  $LC_{\text{relaxed}}$  is the relaxed lattice constant at the current position, and  $LC_{\text{ref}}$  is the lattice constant at the reference position.

Finally, for these concentrations to take effect and all mechanics computations to occur, you must add a short diffusion step if there is none.

During dopant redistribution, the lattice spacing and the lattice mismatch strains are updated, and the doping concentration at the top of the relaxed layer may change. To disable automatic updating of lattice mismatch strains, use:

```
pdbSet Silicon Mechanics UpdateStrain 0
```

To switch off the lattice-spacing tracking at the top of the relaxed layer, use:

```
pdbSet Mechanics LatticeHistory 0
```

## Total Concentration Model

The total concentration model computes the total contribution of lattice mismatch stress with the current impurity concentration and the elastic moduli at the current temperature. For binary compound materials, the elastic moduli are computed with the current mole fraction. With this approach, the lattice mismatch stress is history independent and can change even with an

## 10: Computing Mechanical Stress

### Stress-Causing Mechanisms

unchanged doping profile. The total contribution of lattice mismatch stress is stored in the field `MismatchStress`.

This is the default lattice mismatch model. To switch off this model by computing the lattice mismatch stress increment with the elastic moduli during doping profile change, use the command:

```
pdbSet Mechanics Total.Concentration.Model 0
```

### Reference Concentration Model

The reference concentration model is a simplified lattice mismatch model, which does not distinguish the relaxed region and strained region by specifying the location of the top of the relaxed region. Only the relative concentration accounts for the lattice spacing and the strain changes. For example, the strain in SiGe is:

$$\epsilon = 0.0425 \cdot (C_{\text{Ge}} - C_{\text{ref}}) / C_{\text{Si}} \quad (974)$$

The lattice spacing is computed by  $L_{\text{SiGe}} = L_{\text{Si}} \cdot (1 + \epsilon)$ , where  $C_{\text{Si}}$  is the lattice density of silicon and  $C_{\text{ref}}$  is the reference Ge concentration in SiGe defined by:

```
pdbSet Silicon Germanium Ref.Concentration 1e22
```

The lattice spacing and the strain from this model may not be physical in the relaxed region.

The reference concentration model is used when the structure is flipped for backside processing. To switch on this model, use the command:

```
pdbSet Mechanics Reference.Concentration.Model 1
```

---

## Strained Deposition

Impurity-induced stress can be introduced locally during deposition to account for a lattice-spacing change due to stress rebalancing. For example, the SiGe lattice spacing during unconstrained growth gradually returns to the unconstrained SiGe lattice spacing. The lattice mismatch effect should diminish during the SiGe growth.

The following steps are performed when strained deposition is enabled:

1. Deposit a new layer.
2. Apply a doping profile, and compute the lattice spacing of the newly deposited layer.
3. Set the lattice spacing of the deposited layer to that of the underlayer, and compute the mismatch strain.

4. Perform stress relaxation to establish stress equilibrium, and update the lattice spacing.
5. Merge layers if needed.

To correctly catch the relaxation effect, the thickness of the deposited layer must be chosen properly; a fine mesh is required. Multiple depositions can be particularly useful in such cases.

To switch on the strained deposition model, use the command:

```
pdbSet Mechanics StrainedDeposition 1
```

and specify `Strained.Lattice` in the `deposit` command.

The total concentration model is disabled during strained deposition. The reference concentration model should not be used with strained deposition.

---

## Edge Dislocation

The existence of crystal lattice defects, such as dislocation, affects the channel stress state. The impact of edge dislocation is included by superposing the dislocation-induced stress field for an isotropic infinite medium from elasticity theory. Each edge dislocation can be defined with:

```
stressdata <material> | region=<c>
    apply.dislocation dislocation.origin= {<n> <n> <n>}
    para.orient= {<n> <n> <n>} perp.orient= {<n> <n> <n>} stress.relax
```

where:

- `dislocation.origin` is the location of the dislocation core.
- `para.orient` specifies the direction of the edge dislocation or the direction of the half plane.
- `perp.orient` is the Burgers vector in the perpendicular direction to the half plane. Here, the magnitude of `perp.orient` is the slip distance.
- `stress.relax` switches on the relaxation of stresses after superposing the dislocation-induced stress field.

You must supply either a region name or a material name. If `region` is specified, the stress field is superposed to this region. If a material is specified, the stress field is applied to all regions of crystalline material. To save the edge dislocation geometry information to a TDR file for visualization, specify `saveTDR` with the edge dislocation definition. The edge dislocation is displayed by the half plane of extra atoms. To save the half plane of the missing atoms, use:

```
pdbSet Mechanics Display.Missing.Plane 1
```

## 10: Computing Mechanical Stress

### Stress-Causing Mechanisms

The Burgers vector can be stored in the vector data field `BurgersVector` by setting:

```
pdbSet Mechanics Display.Burgers.Vector 1
```

Singularity exists in the analytic solution at the dislocation core. Without using a nonlinear atomistic theory, the stresses in the core region within a few magnitudes of the Burgers vector to the dislocation core are smoothed away. The factor for this core radius can be defined with:

```
pdbSet Mechanics Dislocation.Coresize.Factor 2.0
```

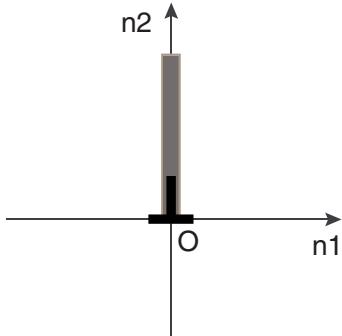


Figure 84 Edge dislocation located at the origin O; n1 is the Burgers vector and n2 is the direction of the half plane

A prototype model for positioning the edge dislocations is available by minimizing the elastic strain energy [1]. The stress field from each edge dislocation is superposed. The elastic strain energy is determined after force equilibrium with edge dislocations at their initial locations.

The initial location of edge dislocation serves as the initial guess and can be defined by:

```
stressdata region=<c> !apply.dislocation dislocation.origin= {<n> <n> <n>}  
para.orient= {<n> <n> <n>} perp.orient= {<n> <n> <n>}
```

where:

- `dislocation.origin` is the initial location of the edge dislocation.
- `!apply.dislocation` is specified to delay applying the dislocation-induced stress field.

Multiple edge dislocations with different Burgers vectors can be defined separately with this syntax.

When all the edge dislocations for minimizing the elastic strain energy are specified, you can start the optimization with the command:

```
stressdata origin.max= {<n> <n> <n>} origin.min= {<n> <n> <n>}  
optimize.dislocation
```

where `origin.max` and `origin.min` define the range of dislocation positions in the specified region. Some additional parameters for optimization convergence control also can be defined in this command (see [stressdata on page 1209](#)).

The movement of edge dislocations depends on the gradient of the total elastic strain energy computed from a discrete integral over all elements. The target of the optimization is set to -5 multiplied by the absolute value of the starting elastic strain energy. This factor can be changed with:

```
pdbSetDouble Mechanics Energy.Optimization.Factor <n>
```

The coordinates of the edge dislocations after optimization are returned in a Tcl list formatted as:

- `<x1> <y1> <x2> <y2> ...` for two dimensions.
- `<x1> <y1> <z1> <x2> <y2> <z2> ...` for three dimensions.

The final stress state remains the same as before the edge dislocations are introduced. The edge dislocations may stop at the local minimum where the elastic strain energy has not reached the global minimum. In such a case, a new optimization step must be started with the initial guess of the edge dislocation positions adjusted based on the previous optimization result. It is also helpful to refine the mesh.

Resolved shear stress can be used to predict the dislocation nucleation. Slip in a grain occurs when the resolved shear stress exceeds the critical value.

The applied stress is resolved along a slip plane in the slip direction where the normal of the slip plane and the slip direction are defined with:

```
stressdata <material> | region=<c> slip.plane.normal= {<n> <n> <n>}  
slip.direction= {<n> <n> <n>}
```

Both vectors are defined with Miller indices in crystal lattices. The actual calculation is switched on with:

```
stressdata resolved.shear.stress
```

This command will output a scalar field `ResolvedShearStress`. This calculation only applies to regions or materials with both the slip plane normal and the slip direction defined.

## Intrinsic Stress

Certain process steps require the deposition of materials with intrinsic stresses. Sentaurus Process can be used to model these process steps. The intrinsic stresses (`StressELXX`, `StressELYY`, `StressELZZ`, `StressELXY`, `StressELYZ`, `StressELZX`) can be prescribed in

## 10: Computing Mechanical Stress

### Stress-Causing Mechanisms

the deposit command (see [deposit on page 928](#)). After stress relaxation, the resulting stresses will be less than the prescribed ones by default. You can scale the prescribed stresses so that for a flat surface, the relaxed stress will be the same as the prescribed stress. To scale the stresses, use the command:

```
pdbSet Mechanics StressRelaxFactor 1
```

For deposition in three dimensions, you can specify stresses in specific layers using the `stressdata` command (see [stressdata on page 1209](#)). For example, the following command sets the *yy* component of the intrinsic stress in the nitride to  $1.4 \times 10^{10}$  dyn/cm<sup>2</sup>:

```
stressdata nitride syyi= 1.4e10
```

For interconnect simulations, intrinsic stresses in metal lines can be modeled as width dependent [2] with either a linear relation or a logarithmic relation, using the parameters defined through the `stressdata` command:

- If modeled as a linear relation, the total intrinsic stresses are given by:

$$\sigma_{xx} = \sigma_{xxi} + \sigma_{xx1} \frac{w_x}{w_b} \quad \sigma_{yy} = \sigma_{yyi} + \sigma_{yy1} \frac{w_y}{w_b} \quad \sigma_{zz} = \sigma_{zzi} + \sigma_{zz1} \frac{w_z}{w_b}$$

- If modeled as a natural logarithmic relation, the total intrinsic stresses are given by:

$$\sigma_{xx} = \sigma_{xxi} + \sigma_{xx2} \ln \frac{w_x}{w_b} \quad \sigma_{yy} = \sigma_{yyi} + \sigma_{yy2} \ln \frac{w_y}{w_b} \quad \sigma_{zz} = \sigma_{zzi} + \sigma_{zz2} \ln \frac{w_z}{w_b}$$

where  $\sigma_{xxi}$ ,  $\sigma_{xx1}$ ,  $\sigma_{xx2}$ ,  $w_b$  are defined through the parameters `sxxi`, `sxx1`, `sxx2`, and base of the `stressdata` command. The other two components (*yy* and *zz*) are defined in the same way, and *w* is calculated internally with respect to the region (not material) boundaries.

The intrinsic stress introduced during material deposition or insertion can also be predefined per material with:

- `stressdata` command options, for example:

```
stressdata <material> deposit.intrinsic sxxi=<n> syyi=<n> szzi=<n> sxyi=<n>
syzi=<n> szxi=<n>
```

The specified material must have been defined and will be checked against the list of existing materials.

- PDB parameters, for example:

```
pdbSetDouble <material> Mechanics Deposit.Intrinsic.StressXX <n>
pdbSetDouble <material> Mechanics Deposit.Intrinsic.StressYY <n>
pdbSetDouble <material> Mechanics Deposit.Intrinsic.StressZZ <n>
pdbSetDouble <material> Mechanics Deposit.Intrinsic.StressXY <n>
pdbSetDouble <material> Mechanics Deposit.Intrinsic.StressYZ <n>
pdbSetDouble <material> Mechanics Deposit.Intrinsic.StressZX <n>
```

There is no syntax check of the material name or the parameter name. The stress unit here is  $\text{dyn}/\text{cm}^2$ .

To omit the above materialwise intrinsic stress definition, use:

```
pdbSet Mechanics Deposit.Intrinsic.Stress 0
```

---

## Stress Rebalancing After Etching and Deposition

When materials are removed from or added to a given structure, physical stress distributions generally change with the corresponding geometry and boundary changes. In simulations, a stress-rebalancing step is required to re-establish the stress equilibrium in the structure and to conform the stress distributions to the new boundaries. By default, a stress-rebalancing operation is called after etching or deposition is performed. To omit the stress-rebalancing step, use:

```
pdbSet Mechanics EtchDepoRelax 0
```

By default, an elastic stress rebalancing is performed irrespective of the materials present. To perform stress rebalancing using other material models, the following PDB parameter must be switched on:

```
pdbSet Mechanics Full.Stress.Update 1
```

If stress balancing is switched on with the `Full.Stress.Update` parameter and inelastic materials (for example, viscoelastic and plastic) are present, a time of 1.0 s is used for the nonlinear simulation. This is equivalent to switching off the stress balancing step and performing a diffuse step for 1.0 s immediately after the etching or deposition step. If a time other than 1.0 s is required for nonlinear material stress balancing, switch off `EtchDepoRelax`, and perform a diffuse step with the time specified.

## Automated Tracing of Stress History

Thermal residual stress in a given device structure is a function of its fabrication history, which consists of process steps at various temperatures and temperature ramps in between. To model stress evolution accurately, all temperature ramps should be traced. When the parameter `StressHistory` is switched on, for example:

```
pdbSet Mechanics StressHistory 1
```

the temperature gaps between process steps such as diffusion, deposition, and etching are detected and filled with instant stress rebalancing, solving for thermal mismatch strains and stresses.

## 10: Computing Mechanical Stress

Sentaurus Process–ParaDiS Application Programming Interface

When stress history is traced and rebalancing is performed, it is done elastically even if inelastic materials are present.

---

## Sentaurus Process–ParaDiS Application Programming Interface

The Parallel Dislocation Simulator (ParaDiS) is a free discrete dislocation dynamics (DDD) simulator originally developed at Lawrence Livermore National Laboratory. ParaDiS can simulate the movement of dislocations in response to the forces imposed by external stress and interdislocation interactions. For the finite simulation domain, the force calculation requires a mechanics solver where Sentaurus Process can be used to generate the bulk mesh and to solve the mechanics equations.

For this coupled simulation, the Sentaurus Process–ParaDiS application programming interface (API) has been developed as a collaboration between Synopsys and the Micro and Nano Mechanics Group at Stanford University led by Dr. Wei Cai. The API is supported in ParaDiS version 2.5.1-SP1.0 or later. The ParaDiS code must be compiled as a shared library (.so file) and dynamically loaded by Sentaurus Process.

The ParaDiS simulation and the Sentaurus Process mechanics solver are coupled in a staggered manner. The coupled simulation is integrated in the `diffuse` command using the following arguments:

- `paradis.control.file`: Specifies the path to the ParaDiS control file that defines the numeric parameters for the DDD simulation, for example, the mobility law.
- `paradis.data.file`: Specifies the path to the ParaDiS data file that defines the simulation domain and the dislocation segments.
- `paradis.library`: Specifies the path to the directory with the shared library file.

All these arguments must be specified in addition to other arguments of the `diffuse` command (see [diffuse on page 935](#)).

The simulation domain must be a single brick-shape homogeneous region. The mechanics boundary conditions on the simulation domain must be defined with the `stressdata` command before the `diffuse` command.

Refer to the ParaDiS documentation for more information about how to create the control file and the data file ([http://micro.stanford.edu/wiki/ParaDiS\\_Manuals](http://micro.stanford.edu/wiki/ParaDiS_Manuals)).

The final configuration of the dislocation network is saved as dislocation segments in a TDR file for visualization. The TDR file also includes the following data fields:

- *Process stress*: External stress from the process steps saved in the nodal field `ProcessStress` and the element field `ProcessStressEL`.
- *Image stress*: Finite-body correction of the dislocation-induced stress saved in the nodal field `ImageStress` and the element field `ImageStressEL`.
- *Dislocation stress*: Infinite-body solution of the dislocation-induced stress saved in the nodal field `DislocationStress` and the element field `DislocationStressEL`.

---

## Saving Stress and Strain Components

By default, stress-tensor components are saved on both elements and nodes. The elastic portions of the strain-tensor components also are saved on both elements and nodes by default. The elastic strains are computed from stresses using isotropic elasticity by default. The anisotropic elasticity also can be used for a given crystalline material when the corresponding `pdb` parameter `Anisotropic` is set. The elastic strain-field computing and saving operation can be omitted using the command:

```
pdbSet Mechanics saveElasticStrain 0
```

The stress tensor can be decomposed and the resulting dilatational and deviatoric stress components can be saved on nodes when the following parameter is switched on:

```
pdbSet Mechanics decomposeStress 1
```

---

## Description of Output Fields

Sentaurus Process assumes that stresses and strains are defined on elements. However, not all tools can read or visualize element values. For this reason, Sentaurus Process performs an element-to-node interpolation of stresses as a postprocessing step and writes both forms of stresses to output.

Element stresses have the prefix `StressEL` and nodal stresses have the prefix `Stress`. The tensor components are given by the suffixes `XX`, `XY`, `YY`, `YZ`, `ZX`, and `ZZ`.

In history-dependent materials, you cannot create a simple closed-form relation between stresses and strains. It is useful, however, to compute the elastic component. The elastic component of the strain is an indicator of the stored strain energy in the system. In addition, the elastic component of the strain is the total strain in elastic materials such as silicon and polysilicon.

## 10: Computing Mechanical Stress

### Saving Stress and Strain Components

Pressure is one-third of the negative of the trace of the stress tensor:

$$P = -\frac{1}{3} \sum_i \sigma_{ii} \quad (975)$$

The field `LatticeSpacing` represents the lattice spacing of the crystal at the location of the node. This is controlled by the presence of lattice-altering species such as germanium or carbon in the structure. In addition, the `strain_profile` command must be specified.

In Sentaurus Process, the `select` command performs Tcl-level and Aligator-level operations. To access the stress components, use the `select` command.

The stresses and strains are represented as symmetric tensors. To access the `xx`, `yy`, and `zz` components of nodal stress values, the variable references for the `select` command are `Stress_xx`, `Stress_yy`, and `Stress_zz`, respectively. To access the `xy`, `yz`, and  `components, use Stress_xy, Stress_yz, and Stress_zx, respectively.`

For element values, the Boolean keyword `element` of the `select` command must be set to `true`. To access the `xx`, `yy`, and `zz` components of the element stress values, the field references for the `select` command are `StressEL_xx`, `StressEL_yy`, and `StressEL_zz`, respectively. To access the `xy`, `yz`, and `zx` components, use `StressEL_xy`, `StressEL_yz`, and `StressEL_zx`, respectively.

[Table 83](#) describes the mechanics-related fields that are defined on elements. [Table 84](#) on page [715](#) describes the mechanics-related fields that are defined on nodes.

Table 83 Fields defined on elements

Field name in Sentaurus Visual	Field name in Sentaurus Process	Description
BaseElasticStrainEL-XX (unitless)	BaseElasticStrainEL_xx (unitless)	XX component of elastic element strain for standard linear solid viscoelasticity model
BaseElasticStrainEL-XY (unitless)	BaseElasticStrainEL_xy (unitless)	XY component of elastic element strain for standard linear solid viscoelasticity model
BaseElasticStrainEL-YY (unitless)	BaseElasticStrainEL_yy (unitless)	YY component of elastic element strain for standard linear solid viscoelasticity model
BaseElasticStrainEL-YZ (unitless)	BaseElasticStrainEL_yz (unitless)	YZ component of elastic element strain for standard linear solid viscoelasticity model
BaseElasticStrainEL-XZ (unitless)	BaseElasticStrainEL_zx (unitless)	ZX component of elastic element strain for standard linear solid viscoelasticity model
BaseElasticStrainEL-ZZ (unitless)	BaseElasticStrainEL_zz (unitless)	ZZ component of elastic element strain for standard linear solid viscoelasticity model

Table 83 Fields defined on elements

Field name in Sentaurus Visual	Field name in Sentaurus Process	Description
BaseStressEL-XX (Pa)	BaseStressEL_xx (dyn/cm <sup>2</sup> )	XX component of elastic element stress for standard linear solid viscoelasticity model
BaseStressEL-XY (Pa)	BaseStressEL_xy (dyn/cm <sup>2</sup> )	XY component of elastic element stress for standard linear solid viscoelasticity model
BaseStressEL-YY (Pa)	BaseStressEL_yy (dyn/cm <sup>2</sup> )	YY component of elastic element stress for standard linear solid viscoelasticity model
BaseStressEL-YZ (Pa)	BaseStressEL_yz (dyn/cm <sup>2</sup> )	YZ component of elastic element stress for standard linear solid viscoelasticity model
BaseStressEL-XZ (Pa)	BaseStressEL_zx (dyn/cm <sup>2</sup> )	ZX component of elastic element stress for standard linear solid viscoelasticity model
BaseStressEL-ZZ (Pa)	BaseStressEL_zz (dyn/cm <sup>2</sup> )	ZZ component of elastic element stress for standard linear solid viscoelasticity model
StressEL-XX (Pa)	StressEL_xx (dyn/cm <sup>2</sup> )	XX component of element stress
StressEL-XY (Pa)	StressEL_xy (dyn/cm <sup>2</sup> )	XY component of element stress
StressEL-YY (Pa)	StressEL_yy (dyn/cm <sup>2</sup> )	YY component of element stress
StressEL-YZ (Pa)	StressEL_yz (dyn/cm <sup>2</sup> )	YZ component of element stress
StressEL-XZ (Pa)	StressEL_zx (dyn/cm <sup>2</sup> )	ZX component of element stress
StressEL-ZZ (Pa)	StressEL_zz (dyn/cm <sup>2</sup> )	ZZ component of element stress

Table 84 Fields defined on nodes

Field name in Sentaurus Visual	Field name in Sentaurus Process	Description
Displacement-X (um)	Displacement_x (cm)	X-component of displacement
Displacement-Y (um)	Displacement_y (cm)	Y-component of displacement
Displacement-Z (um)	Displacement_z (cm)	Z-component of displacement
ElasticEnergyDens (J/m <sup>3</sup> )	ElasticEnergyDens (erg/cm <sup>3</sup> )	Elastic strain energy density
ElasticStrain-XX (unitless)	ElasticStrain_xx (unitless)	XX component of elastic strain
ElasticStrain-XY (unitless)	ElasticStrain_xy (unitless)	XY component of elastic strain

## 10: Computing Mechanical Stress

### Saving Stress and Strain Components

Table 84 Fields defined on nodes

Field name in Sentaurus Visual	Field name in Sentaurus Process	Description
ElasticStrain-YY (unitless)	ElasticStrain_YY (unitless)	YY component of elastic strain
ElasticStrain-YZ (unitless)	ElasticStrain_yz (unitless)	YZ component of elastic strain
ElasticStrain-XZ (unitless)	ElasticStrain_zx (unitless)	ZX component of elastic strain
ElasticStrain-ZZ (unitless)	ElasticStrain_zz (unitless)	ZZ component of elastic strain
LatticeSpacing (cm)	LatticeSpacing (cm)	Lattice spacing
MisesStress (Pa)	MisesStress (dyn/cm <sup>2</sup> )	von Mises stress
Pressure (Pa)	Pressure (dyn/cm <sup>2</sup> )	Pressure
Stress-XX (Pa)	Stress_xx (dyn/cm <sup>2</sup> )	XX component of node stress
Stress-XY (Pa)	Stress_xy (dyn/cm <sup>2</sup> )	XY component of node stress
Stress-YY (Pa)	Stress_yy (dyn/cm <sup>2</sup> )	YY component of node stress
Stress-YZ (Pa)	Stress_yz (dyn/cm <sup>2</sup> )	YZ component of node stress
Stress-XZ (Pa)	Stress_zx (dyn/cm <sup>2</sup> )	ZX component of node stress
Stress-ZZ (Pa)	Stress_zz (dyn/cm <sup>2</sup> )	ZZ component of node stress

**NOTE** The stresses and strains in the output file are according to the unified coordinate system (UCS).

Table 85 lists the mechanics-related fields available for use in the select command.

Table 85 Fields available in select command

Field type	Field name		
Displacement	Displacement_x	Displacement_y	Displacement_z
	StepDisplacement_x	StepDisplacement_y	StepDisplacement_z

Table 85 Fields available in select command

Field type	Field name		
Stress	StressEL_xx	StressEL_yy	StressEL_zz
	StressEL_xy	StressEL_yz	StressEL_zx
	MisesStress	Pressure	
	PrincipalStress1	PrincipalStress2	PrincipalStress3
	Stress_xx	Stress_yy	Stress_zz
	Stress_xy	Stress_yz	Stress_zx
Strain	ElasticStrainEL_xx	ElasticStrainEL_yy	ElasticStrainEL_zz
	ElasticStrainEL_xy	ElasticStrainEL_yz	ElasticStrainEL_zx
	PlasticStrainEL_xx	PlasticStrainEL_yy	PlasticStrainEL_zz
	PlasticStrainEL_xy	PlasticStrainEL_yz	PlasticStrainEL_zx
	ViscoPlasticStrainEL_xx	ViscoPlasticStrainEL_yy	ViscoPlasticStrainEL_zz
	ViscoPlasticStrainEL_xy	ViscoPlasticStrainEL_yz	ViscoPlasticStrainEL_zx
	ElasticStrain_xx	ElasticStrain_yy	ElasticStrain_zz
	ElasticStrain_xy	ElasticStrain_yz	ElasticStrain_zx

## Tracking Maximum Stresses

During a typical process flow, the maximum stresses may be reached in a process step and, subsequently, the stresses may fall. If the material is prone to failure through delamination or nucleation of dislocations, the failure may occur when the maximum stress is reached.

To always track the maximum stresses, set the following parameter:

```
pdbSet Mechanics SaveMaxStress 1
```

The **StressMaxEL** field is updated when the current stress is greater than the stored stress. In this way, the maximum is maintained throughout the process flow. The maximum element stresses and the von Mises stress are computed and stored.

Using the **stressdata** command (see [stressdata on page 1209](#)), a list of maximum stresses (hot spots) and their locations can be obtained. The hot spots can be evaluated by one of the six stress components (sxx, syy, szz, sxy, syz, and szx), the von Mises stress, or the hydrostatic stress (negative pressure value or the pressure). The command returns a list of maximum stress values (largest magnitude, largest tensile, largest compressive) and the corresponding location coordinates.

## Principal Stresses

Principal stresses are normal stresses that act on the planes where shear stresses are zero, that is:

$$(\sigma - \sigma_p I) \hat{n} = 0 \quad (976)$$

which implies that the determinant of the Cauchy relation in matrix form is zero:

$$\sigma_p^3 - I_1 \sigma_p^2 + I_2 \sigma_p - I_3 = 0 \quad (977)$$

where the coefficients are known as the three stress invariants:

$$\begin{aligned}\sigma_1 &= \sigma_{ii} \\ \sigma_2 &= \frac{1}{2}(\sigma_{ii}\sigma_{jj} - \sigma_{ij}\sigma_{ji}) \\ \sigma_3 &= \det(\sigma_{ij})\end{aligned} \quad (978)$$

The three principal stresses are ordered from the largest tensile (positive) stress to the largest compressive (negative) stress, and are named:

- First principal stress:  $\sigma_1 = \max(\sigma_{p1}, \sigma_{p2}, \sigma_{p3})$
- Second principal stress:  $\sigma_2 = I_1 - \sigma_1 - \sigma_3$
- Third principal stress:  $\sigma_3 = \min(\sigma_{p1}, \sigma_{p2}, \sigma_{p3})$

The first and third principal stresses are also algebraically the largest and the smallest normal stresses that can be found at this point. Therefore, principal stresses are often adopted as measures to evaluate the integrity of structures.

To calculate the principal stresses, use:

```
pdbSet Mechanics Calculate.Principal.Stress 1
```

The resulting fields are:

- PrincipalStress1 for the first principal stress.
- PrincipalStress2 for the second principal stress.
- PrincipalStress3 for the third principal stress.

If the maximum-stress tracking flag is switched on:

```
pdbSet Mechanics SaveMaxStress 1
```

Sentaurus Process also tracks the maximum principal stresses that occurred during the entire simulation process and stores them as:

- PrincipalStress1Max
- PrincipalStress2Max
- PrincipalStress3Max

## Principal Strains

Principal strains are normal strains that act on the planes where shear strains are zero, that is:

$$(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_p \mathbf{I}) \hat{\mathbf{n}} = 0 \quad (979)$$

which implies that the determinant of the Cauchy relation in matrix form is zero:

$$\varepsilon_p^3 - I_1 \varepsilon_p^2 + I_2 \varepsilon_p - I_3 = 0 \quad (980)$$

where the coefficients are known as the three strain invariants:

$$\begin{aligned} \varepsilon_1 &= \varepsilon_{ii} \\ \varepsilon_2 &= \frac{1}{2}(\varepsilon_{ii}\varepsilon_{jj} - \varepsilon_{ij}\varepsilon_{ji}) \\ \varepsilon_3 &= \det(\varepsilon_{ij}) \end{aligned} \quad (981)$$

The three principal strains are ordered from the largest tensile (positive) strain to the largest compressive (negative) strain, and are named:

- First principal strain:  $\varepsilon_1 = \max(\varepsilon_{p1}, \varepsilon_{p2}, \varepsilon_{p3})$
- Second principal strain:  $\varepsilon_2 = I_1 - \varepsilon_1 - \varepsilon_3$
- Third principal strain:  $\varepsilon_3 = \min(\varepsilon_{p1}, \varepsilon_{p2}, \varepsilon_{p3})$

The first and third principal strains are also algebraically the largest and the smallest normal strains that can be found at this point.

To calculate the principal strains, use:

```
pdbSet Mechanics Calculate.Principal.Strain 1
```

The resulting fields are:

- PrincipalStrain1 for the first principal strain.
- PrincipalStrain2 for the second principal strain.
- PrincipalStrain3 for the third principal strain.

## 10: Computing Mechanical Stress

### References

If the maximum-stress tracking flag is switched on:

```
pdbSet Mechanics SaveMaxStress 1
```

Sentaurus Process also tracks the maximum principal strains that occurred during the entire simulation process and stores them as:

- PrincipalStrain1Max
- PrincipalStrain2Max
- PrincipalStrain3Max

---

## Nodal Stress and Strain at Like-Material Interface

Nodal stress and strain data fields are interpolated regionwise from the corresponding element data fields. They are discontinuous across the interfaces of different materials. At the interface of like materials, the nodal fields `Pressure` and `ElasticStrain` are specially interpolated to have a continuous distribution. This list of nodal data fields can be changed with:

```
pdbSet Mechanics Like.Material Boundary Continuous {<list of fields>}
```

Each like-material interface can have its own list of continuous nodal data fields, for example:

```
pdbSetString <mat1_mat2> Mechanics Boundary Continuous {<list of fields>}
```

---

## References

- [1] R. Gatti *et al.*, “Dislocation engineering in SiGe heteroepitaxial films on patterned Si (001) substrates,” *Applied Physics Letters*, vol. 98, no. 12, p. 121908, 2011.
- [2] Y.-C. Joo, J.-M. Paik, and J.-K. Jung, “Effect of Microstructure and Dielectric Materials on Stress-Induced Damages in Damascene Cu/Low-k Interconnects,” in *MRS Symposium Proceedings, Materials, Technology and Reliability of Advanced Interconnects*, vol. 863, San Francisco, CA, USA, p. B7.6/O11.6, March 2005.

# CHAPTER 11 Mesh Generation

---

*This chapter describes the mesh algorithms and meshing parameters available in Sentaurus Process.*

---

## Overview

Sentaurus Process automatically generates meshes as they are needed. The behavior of the automatic-meshing scheme differs depending on the dimension of the simulation because of the time required to generate meshes. In one dimension and two dimensions, meshes are generated after every geometry operation such as etching and deposition. In three dimensions, meshes are only generated immediately before steps that require a bulk mesh, such as a `diffuse` or an `implant` command, and structure saving. This scheme can reduce the time spent when there are multiple geometry-changing steps without a `diffuse` or an `implant` command (or any other step requiring a mesh) in between.

Sentaurus Process uses Sentaurus Mesh as its meshing engine. Since Sentaurus Mesh is a suite of tools, when discussing its different meshing algorithms, for simplification, *Sentaurus Mesh* will be used in this chapter.

The mesh generation process starts with a bisection algorithm, which places mesh points as instructed by the user. Afterwards, the mesh elements are created using a modified Delaunay-meshing algorithm. Refer to the [Sentaurus™ Mesh User Guide](#) for details.

The meshes generated within Sentaurus Process can be refined adaptively, statically, or as a combination of adaptive and static refinements. The refinement can be specified using one of the major types of refinement box:

- Field based (adaptive meshing)
- Mask based
- Uniform (standard)
- Interface axis-aligned
- Interface offsetting (offset normal to the interface)

All these refinement types are user controllable. In addition, Sentaurus Mesh enforces mesh smoothing to limit the changes in element size from one element to the next. This smoothing is important for mechanics accuracy and convergence behavior (see [Mesh Refinement on page 722](#)).

## 11: Mesh Generation

### Overview

One important algorithm affecting refinement behavior is the `UseLines` algorithm. This algorithm inserts lines created using the `line` command into the internal bisection algorithm before any other lines are introduced. Further mesh refinement proceeds by bisecting the boxes created by the `UseLines` lines. This has the effect of isolating static regions of a structure from regions where the boundaries are moving due to geometric operations. Geometry movement naturally causes perturbations to the mesh lines. The `UseLines` lines compartmentalize this mesh movement to minimize solution degradation from interpolation. See [UseLines: Keeping User-Defined Mesh Lines on page 756](#).

**NOTE** Because the bisection algorithm in Sentaurus Process differs from the one used to create mesh refinement in the standalone Sentaurus Mesh tool, it is not possible to create meshes identical to those created with Sentaurus Mesh. However, element quality, stability, and the Delaunay properties should be qualitatively the same.

---

## Mesh Refinement

Mesh refinement is a two-step process:

- First, you define the refinement box.
- Second, the mesh is refined when the next remesh occurs either with an explicit `grid remesh` call or during standard geometry modifications such as etch, deposit, clip, or native layer formation.

The refinement boxes remain valid unless the list of refinement boxes is cleared with the `refinebox clear` command.

All refinement boxes have refinement criteria that add mesh and constraints that can be used to spatially limit where the mesh refinement occurs. One type of mesh refinement criteria is available for each type of refinement box, and the criteria essentially define the box type. The mesh refinement criteria and, therefore, the refinement box type can be either static or adaptive. All types of refinement box can be mixed in a command file as required.

**NOTE** Only one type of mesh refinement must be defined in one `refinebox` command.

The refinement box spatial constraints are specified along with the mesh refinement criteria in the `refinebox` command and can be combined in one command.

The spatial constraints available include:

- A material constraint using the `materials` argument that takes a list of materials.
- Region constraints using the `regions` argument that takes a list of region names.
- The `min` and `max` arguments that limit the size of the refinement box (which by default applies to all of the space).
- A mask constraint using the `mask`, `extrusion.min`, and `extrusion.max` arguments that limit the size of the refinement box.

Refinement information also can be extracted and written to a file readable by Sentaurus Mesh using the `mshcmd` flag in conjunction with the `tdr` or `tdr.bnd` argument of the `struct` command (see [struct on page 1217](#)).

---

## Viewing Mesh Refinement

To aid in setting mesh refinement, you can store the current minimum edge length in each direction as a field using the command:

```
pdbSet Grid Set.Min.Edge 1
```

When specified, Sentaurus Process computes the smallest edge length in each direction and saves it in three fields:

- `MinXEdgeLength`
- `MinYEdgeLength` (for 2D or 3D structures)
- `MinZEdgeLength` (for 3D structures)

In addition, it prints the average edge length to the screen.

---

## Static Mesh Refinement

This section discusses static (not adaptive) mesh refinement.

---

### Standard Refinement Boxes

The standard refinement box allows you to specify a smoothly varying mesh density inside the refinement box at three locations in the x-, y- and z-directions using the `xrefine`, `yrefine`, and `zrefine` parameter lists, respectively.

Each of the `xrefine`, `yrefine`, and `zrefine` parameters lists can contain from one to three values. If all three `xrefine`, `yrefine`, and `zrefine` values are specified, the mesh density varies quadratically in that direction. If two are specified, the variation is linear from top to bottom. If only one value is specified, a constant mesh density is assumed.

This example specifies two refinement boxes and performs a remesh:

```
refinebox min= {-0.25 0.4 0.0} max= {0.4 0.6 1.0} xrefine= {0.1 0.06 0.1} \
    yrefine= {0.1 0.01 0.1} zrefine = {0.01} oxide
refinebox min= {0.6 0.6} max= {0.8 0.8} xrefine= 0.1 silicon
grid remesh
```

The first refinement box only applies to oxides within the cube delimited by  $-0.25 \leq x \leq 0.4$ ,  $0.4 \leq y \leq 0.6$ ,  $0.0 \leq z \leq 1.0$ . It specifies a quadratically varying mesh density for x and y, and a constant mesh density for z.

**NOTE** Calculating the linear or quadratic variation of the mesh density when two or three x-, y-, or z-direction values are given requires the specification of `min` and `max`. If `min` and `max` are not specified and at least one region is specified, the minimum and maximum values of the bounding box for that region serve as `min` and `max` for the calculation. If more than one region is specified, only the bounding box of the first region is used for the calculation, although all regions are used as constraints to the refinement.

---

## Interface Axis-Aligned Refinement Boxes

Refinement near interfaces can be specified globally or constrained spatially inside a refinement box using the `refinebox` command. So it is possible to have a large global default minimum interface mesh-spacing, for example, and a smaller localized value inside a box. The parameters affecting interface refinement are demonstrated in the following examples:

- Set the global mesh criteria near interfaces. This is the maximum size the first normal edge can be, and it is possible for the edge to be `0.5 min.normal.size`:

```
pdbSet Grid SnMesh min.normal.size <n>
```

- Set the global growth rate of the edge size away from interfaces:

```
pdbSet Grid SnMesh normal.growth.ratio.2d <n>
pdbSet Grid SnMesh normal.growth.ratio.3d <n>
```

- To constrain the interface mesh specification to a particular set of materials or material interfaces, set `min.normal.size`, or `normal.growth.ratio`, or both locally within a refinement box:

```
refinebox min.normal.size=<n> normal.growth.ratio=<n>
[interface.materials= <list> | interface.mat.pairs= <list>]
```

---

## Interface Offsetting Refinement Boxes

In addition, the Sentaurus Mesh offsetting algorithm can be used to create offsetting layers that are conformal to the interface rather than aligned to the coordinate axes by specifying the `offsetting` keyword, which also permits regionwise interface specification in addition to the materialwise possibility:

```
refinebox offsetting min.normal.size=<n> normal.growth.ratio=<n>
[interface.materials= <list> | interface.mat.pairs= <list>]
[interface.regions= <list> | interface.region.pairs= <list>]
```

For Sentaurus Mesh offsetting, an additional argument `offsetting.maxlevel=<i>` defines the number of layers to be generated at the interface. It can be defined globally through the PDB parameter `Grid SnMesh offsetting.maxlevel`, or on a materialwise or regionwise basis using the `refinebox` command as shown in the following possibilities:

```
pdbSet Grid SnMesh offsetting.maxlevel <i>
refinebox offsetting.maxlevel=<i> interface.materials= <list>
refinebox offsetting.maxlevel=<i> interface.regions= <list>
```

**NOTE** For Sentaurus Mesh offsetting, `offsetting.maxlevel` can only be defined on a material or region basis with `interface.materials` or `interface.regions` or globally, not with `interface.mat.pairs` or `interface.region.pairs`.

**NOTE** For Sentaurus Mesh offsetting, `min.normal.size` and `normal.growth.ratio` can only be defined by material pair or region pair with `interface.mat.pairs` or `interface.region.pairs` or globally, not with `interface.materials` or `interface.regions`.

Offset-meshing parameters defined at interfaces using `interface.mat.pairs` or `interface.region.pairs` are interpreted in a symmetric way by default. This means that, given the specification of a material or region pair  $x_1/x_2$ , the parameters are defined for both  $x_1$  at the  $x_2$  interface and  $x_2$  at the  $x_1$  interface. If `!double.side` is given, Sentaurus Mesh interprets  $x_1/x_2$  in a nonsymmetric way, that is, only for  $x_1$  at the  $x_2$  interface.

---

## Refinement Inside a Mask

Mask-based refinements are similar to standard refinements (see [Standard Refinement Boxes on page 723](#)), except that they have an additional constraint that is defined by a volume specified by a previously existing mask. This constraint is applied in addition to the normal box

constraint defined by the `min` and `max` parameters. Mask-based refinements are a way to have layout-driven refinements.

For example, if you specify `min` and `max`, the refinement area will be the intersection of the specified rectangle and the mask. If you specify a material name, the final refinement will be the intersection of the regions with such a material and the mask.

These constraints are specified using the `refinebox` command with the following options:

- A mask name (`mask`).
- Minimum and maximum coordinates in the `x`-direction where the refinement will be applied (`extrusion.min` and `extrusion.max`).
- An optional parameter to see whether the refinement should extend some distance away from the mask (`extend`).

Negative masks are also allowed. Mask boundaries are never interpreted as being infinite in any direction, even if they extend far from the simulation boundary. Consequently, *shrinking* a refinement by specifying a negative extension parameter might leave a region uncovered, even if the mask originally extended past the boundary. For example, if a mask from (-0.010 to 1) covers a domain from (0 to 2), specifying `extend=-0.02` will produce a refinement extending from (0.010 to 0.98), thereby leaving the region from 0 to 0.010 unrefined.

### Example

First, create a mask, and then a refinement box can be issued:

```
polygon name= pol segments= { -0.5 -0.5 -.25 -.5 -.25 -.05 .25 -.05 .25 -.5 \
    .5 -.5 .5 0 -.5 0 }
mask name= "Mask" polygons= {pol}

# Now that there is a mask, it can be used to produce a refinement.
refinebox name= "refi_mask" mask= "Mask" xrefine= { .075 .075 .075 } \
    yrefine= { .075 .075 .075 } extrusion.min= 0 extrusion.max= 0.05 \
    extend= -0.1
```

---

## Refinement Near Mask Edges or Mask Corners

Refinement also can be constrained to be near mask edges or mask corners. The following arguments are available in the `refinebox` command:

- For mask edge-based refinement:
  - `mask.edge.refine.extent`
  - `mask.edge.mns`
  - `mask.edge.ngn`

- For mask corner-based refinement:

- `mask.corner.refine.extent`
- `mask.corner.mns`
- `mask.corner.ngr`

The `mask.edge.refine.extent` argument must be specified to switch on mask edge-based refinement and to set the lateral extent of the refinement from the mask edge. Vertically, the mask edge-based refinement can be controlled with the x-coordinate of the `min` and `max` arguments. The minimum mesh spacing near the mask edge is set with `mask.edge.mns` (the default is taken from the PDB parameter `Grid SnMesh min.normal.size`), and the growth of the edge length away from the mask edge is specified with `mask.edge.ngr` (default is 1.0, meaning the constant edges of lengths `mask.edge.mns` in the normal direction).

Equivalently, the `mask.corner.refine.extent` argument must be specified to switch on mask corner-based refinement and to set the lateral extent of the refinement from the mask corner. Vertically, the mask corner-based refinement can be controlled with the x-coordinate of the `min` and `max` arguments. The minimum mesh spacing near the mask corner is set with `mask.corner.mns` (the default is taken from the PDB parameter `Grid SnMesh min.normal.size`), and the growth of the edge length away from the mask corner is specified with `mask.corner.ngr` (default is 1.0, meaning the constant edges of lengths `mask.corner.mns` in the normal direction).

**NOTE** Similar to the PDB parameter `Grid SnMesh min.normal.size`, actual edge lengths may be up to two times smaller than `mask.edge.mns` or `mask.corner.mns` at the mask edge or mask corner, respectively, because of the binary-tree refinement algorithm.

**NOTE** The `refinebox` command can specify either mask edge-based refinement, or mask corner-based refinement, or both at the same time.

An example of using mask edge-based refinement is:

```

polygon name= p1 segments= {1.0 1.0 1.0 5.0 3.0 5.0 3.0 2.5 2.0 2.5 2.0 1.0}
mask name= m1 polygons= p1

refinebox clear

# Prevent mesh propagation by defining regular coarse mesh
refinebox yrefine= 0.5 zrefine= 0.5

# Add edge-based refinement
refinebox mask= m1 mask.edge.mns= 0.08 mask.edge.refine.extent= 0.25

grid remesh

```

The resist layer was created later using the command:

```
photo mask= m1 thickness= 0.05
```

[Figure 85](#) shows the result.

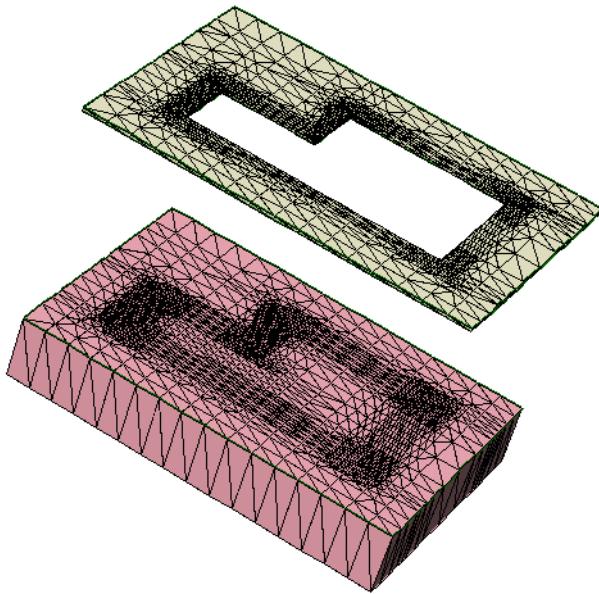


Figure 85 Mask edge-based refinement shown on the mask and in silicon

---

## Uniform Mesh Scaling

Often in simulations, uniform mesh refinement is required to study mesh effects or convergence. After defining all of the other mesh refinement criteria, the mesh can be further split uniformly by a specified factor in each direction. This is achieved by a final split of the binary tree used in refinement.

To scale a mesh by a specified factor, you can use the `binarytree.split.factor.x`, `binarytree.split.factor.y`, and `binarytree.split.factor.z` parameters, for example:

```
pdbSet Grid SnMesh binarytree.split.factor.x 4  
pdbSet Grid SnMesh binarytree.split.factor.y 2  
pdbSet Grid SnMesh binarytree.split.factor.z 1  
  
grid remesh
```

In this example, the final mesh is refined by a factor of 4 in the x-direction and a factor of 2 in the y-direction, resulting in approximately 8 times more elements.

**NOTE** The split factors must be specified in powers of 2.

In addition, you can apply the split factors over a specified box, which is defined in two dimensions by:

```
pdbSet Grid SnMesh binarytree.split.box {xmin 0.0 ymin 0.0 xmax 0.0 ymax 0.0}
```

and, in three dimensions by:

```
pdbSet Grid SnMesh binarytree.split.box {xmin 0.0 ymin 0.0 zmin 0.0 xmax 0.0 \
ymax 0.0 zmax 0.0}
```

---

## Adaptive Mesh Refinement

Tailoring a mesh to a specific problem with static refinement boxes can be tedious and time-consuming. In addition, for some applications, dopant profiles evolve so much during the process that the areas where a finer mesh was needed at the beginning are very different from the areas where a finer mesh is needed at the end.

To accurately capture the entire evolution with a static mesh, it is necessary to put a fine mesh over large areas of the structure leading to long simulation times and large memory use. Adaptive meshing in Sentaurus Process addresses these issues.

The adaptive-meshing feature has a major component: field-based refinement.

For details, see [Tips for Adaptive Meshing on page 739](#).

Adaptive implantation for field-based refinement uses the same refinement parameters and criteria. When adaptive meshing is switched on, field-based refinement is performed during every remesh step and for any dimension. This happens for all etching, deposition, implantation, native layer, regrid, and transform operations. In addition, during time-stepping at a specified step interval, a check of the current mesh is made to determine whether a remesh is required; then the remesh is performed if necessary. For details, see [Adaptive Meshing During Diffusion on page 737](#).

Finally, when adaptive meshing is used during implantation, in addition to adaptively refining the newly implanted species and damage, adaptive refinement (also based on existing fields) is applied simultaneously.

---

## Adaptive Refinement Criteria

Numerous refinement functions are available to deal with differing fields and situations. All functions involve some comparison between values on neighboring nodes and possible values between neighboring nodes. In some cases, the same refinement function is available in Sentaurus Mesh, and similar results to Sentaurus Mesh refinement will be obtained. The following refinement criteria are available:

- Relative difference (default)
- Absolute difference
- Logarithmic difference
- Inverse hyperbolic sine (asinh) difference
- Gradient
- Local dose error
- Interval refinement

These refinements can be applied globally (default) or they can be limited as follows:

- Boxwise
- Materialwise
- Regionwise

Detailed descriptions of the refinement types, their respective control parameters, and instructions for applying refinement constraints are given in subsequent sections. The default adaptive meshing parameters have been set to apply only relative difference criteria to the entire structure, and they typically produce a fairly coarse mesh. It is necessary to set one criterion or more to produce a mesh sufficiently fine to reach a required accuracy.

Adaptive meshing is switched off by default. To switch on adaptive meshing, use:

```
adbSet Grid Adaptive 1  
adbSet Grid SnMesh UseLines 1 ;# Recommended with adaptive meshing
```

### Relative Difference Criteria

The relative difference between two neighboring nodes is computed as follows:

$$2 \frac{|C_1 - C_2|}{(C_1 + C_2 + \alpha)} \quad (982)$$

where  $C_i$  is the field value on node  $i$ , and  $\alpha$  is the field-specific refinement parameter set with:

```
adbSet Grid <Field> Refine.Abs.Error <n>
```

or `def.abs.error` and `abs.error`, which are parameters of the `refinebox` command.

If the value of the expression in Eq. 982 is greater than the maximum relative difference, the edge between node 1 and node 2 is split. To set the maximum relative difference, use:

```
pdbSet Grid <Field> Refine.Rel.Error <n>
```

or `def.rel.error` and `rel.error`, which are parameters of the `refinebox` command.

The quantity `<Field>` is the name of the field, and `<n>` is a unitless number for `Refine.Rel.Error` and `Refine.Abs.Error`; the units are the same as those of the field. The default values for `Refine.Abs.Error` and `Refine.Rel.Error` are set from `<Field> = AdaptiveField`, except for the standard dopants, point defects, and Damage that have entries in the Parameter Database (PDB).

The density of the mesh is sensitive to `Refine.Rel.Error` because it represents the target relative change of the field across an edge. For many standard situations, a number of the order of 1.25 gives a coarse mesh, and a number of approximately 0.5 often gives a fine mesh. The parameter  $\alpha$  sets a smooth cutoff such that values of the field below  $\alpha$  result in no refinement.

**NOTE** The relative difference criteria must only be used with fields that are always positive.

## Absolute Difference Criteria

The absolute difference between two neighboring nodes is computed simply:

$$|C_1 - C_2| \tag{983}$$

where  $C_i$  is the field value on node  $i$ . If the value of the expression in Eq. 983 is greater than the maximum absolute difference, the edge between nodes 1 and 2 is split. The maximum allowable absolute difference can be set with:

```
pdbSet Grid <Field> Refine.Max.Difference <n>
```

## Logarithmic Difference Criteria

The logarithmic (base 10) difference between two neighboring nodes is computed as follows:

$$|\log(C_1 + \alpha) - \log(C_2 + \alpha)| \tag{984}$$

where  $C_i$  is the field value on node  $i$ , and  $\alpha$  is the low value cutoff that can be set with:

```
pdbSet Grid <Field> Refine.Abs.Error <n>
```

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### Adaptive Mesh Refinement

or `def.abs.error` and `abs.error`, which are parameters of the `refinebox` command.

If the value of the expression in Eq. 984 is greater than the maximum logarithmic difference, the edge between nodes 1 and 2 is split. To set the maximum logarithmic difference, use:

```
pdbSet Grid <Field> Refine.Max.LogDiff <n>
```

or `def.max.logdiff` and `max.logdiff`, which are parameters of the `refinebox` command.

**NOTE** The logarithmic difference criteria must only be used with fields that are always positive. Use the inverse hyperbolic sine (`asinh`) difference criteria for fields that can have negative values such as stresses.

## Inverse Hyperbolic Sine (`asinh`) Difference Criteria

The `asinh` difference between two neighboring nodes is computed as follows:

$$|\operatorname{asinh}(C_1) - \operatorname{asinh}(C_2)| \quad (985)$$

where  $C_i$  is the field value on node  $i$ . If the value of the expression in Eq. 985 is greater than the maximum `asinh` difference, the edge between nodes 1 and 2 is split. To set the maximum `asinh` difference, use:

```
pdbSet Grid <Field> Refine.Max.AsinhDiff <n>
```

or `def.max.asinhdiff` and `max.asinhdiff`, which are parameters of the `refinebox` command.

## Gradient Criteria

The gradient between two neighboring nodes is computed as follows:

$$\frac{|C_1 - C_2|}{l_{12}} \quad (986)$$

where  $C_i$  is the field value on node  $i$ , and  $l_{ij}$  is the length of the edge between nodes  $i$  and  $j$ . If the value of the expression in Eq. 986 is greater than the maximum gradient, the edge between the two nodes is split. To set the maximum gradient, use:

```
pdbSet Grid <Field> Refine.Max.Gradient <n>
```

or `def.max.gradient` and `max.gradient`, which are parameters of the `refinebox` command.

## Local Dose Error Criteria

If an edge between two neighboring nodes is not split, the local dose error is computed as follows:

$$|0.5C_{12} - 0.25C_i - 0.25C_j|l_{ij}s_{ij} \quad (987)$$

where:

- $C_i$  is the field value on node  $i$ .
- $C_{ij}$  is the concentration at the midpoint between nodes  $i$  and  $j$ .
- $l_{ij}$  is the length of the edge between nodes  $i$  and  $j$ .
- $s_{ij}$  is the box size perpendicular to the edge between nodes  $i$  and  $j$  (see [Figure 86](#)).

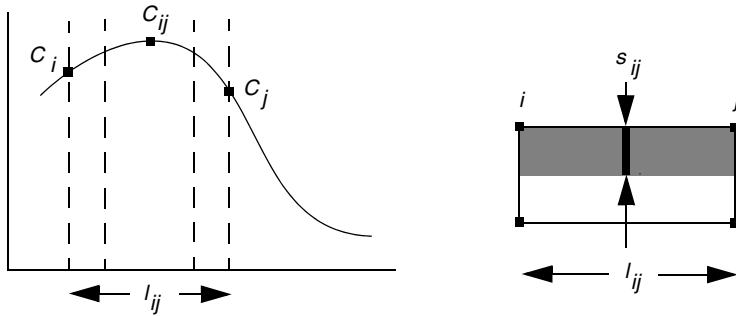


Figure 86 (Left) One-dimensional and (right) 2D representation of dose loss criteria

The function in [Figure 86 \(left\)](#) is taken from the previous mesh (or from an analytic implantation). The box with four points in [Figure 86 \(right\)](#) represents one cell of the mesh refinement tree. The shaded area is the part of the 2D field under consideration. The dose in the shaded area is computed in two ways:

- As is
- If the edge between  $i$  and  $j$  is split

If the difference between these two ways is greater than `max.dose.error`, the edge is split.

The box size is 1.0 (unitless) in 1D; it is the box width (in cm) in 2D; and it is the box area ( $\text{cm}^{-2}$ ) perpendicular to the edge  $i-j$  in 3D. If the value of the expression in [Eq. 987](#) is greater than the normalized maximum local dose error, the edge between the two nodes is split. The local dose error can be set with:

```
pbSet Grid <Field> Refine.Max.DoseError <n>
```

where  $<n>$  has units of  $\text{cm}^{-2}$ , or `def.max.dose.error` and `max.dose.error`, which are parameters of the `refinebox` command.

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The local dose error is first multiplied by the simulation size before comparing it to the expression in Eq. 987. The simulation size is 1.0 (unitless) in 1D, the simulation width (in cm) in 2D, and the simulation lateral area in 3D (in  $\text{cm}^{-2}$ ).

To estimate the total dose loss, you must estimate how many nodes carry a significant concentration of the field in question and then multiply that number by the local dose error to obtain approximately the maximum total dose error expected. (In practice, the dose error is often considerably less than this.) This quantity is relatively easy to understand and is less sensitive than some other parameters to process conditions.

## Interval Refinement Criteria

Interval refinement provides a way to refine the mesh such that field values within a certain interval are well resolved. Interval refinement produces mesh edges of a specified length wherever the field values are within a specified interval. Four parameters are required to define an interval refinement:

- A minimum and maximum value
- $C_{\min}$  and  $C_{\max}$
- A target length,  $l_t$
- A target length scaling,  $s$

To preserve the anisotropy of the mesh, interval refinement examines each edge of a refinement cell and calculates an effective edge length  $l_{\text{eff}}$  defined by:

$$l_{\text{eff}} = \text{abs}((r_1 - r_2) \cdot \nabla C) \quad (988)$$

where  $r_1$  and  $r_2$  are the endpoints of the edge, and  $\nabla C$  is the average gradient of the field in the refinement cell. Edges that are nearly parallel to the contours of the field have effective edge lengths near zero. Edges that are nearly perpendicular to the contours have effective edge lengths near their actual edge length. Since edges are split only when they are longer than a given target length, edges that are parallel to the field contours are allowed to be longer than those that are perpendicular.

Interval refinement will split any edge whose effective edge length exceeds the effective target length. The effective target length is calculated differently depending on whether the field values on the edge overlap the interval specified by  $C_{\min}$  (`refinebox min.value`) and  $C_{\max}$  (`refinebox max.value`).

Let  $C_1$  and  $C_2$  be the values of the field on the endpoints of the edge. If the relation  $C_{\max} > C > C_{\min}$  is satisfied for any value of  $C$  between  $C_1$  and  $C_2$ , the edge overlaps the interval.

For edges that overlap the interval, the effective target length is exactly the target length that you specify (`refinebox target.length`), that is:

$$lt_{\text{eff}} = lt \quad (989)$$

For edges that do not overlap:

$$lt_{\text{eff}} = lt(1 + \log C_a - \log C_b)^2 s \quad (990)$$

where  $C_a$  is either  $C_{\min}$  or  $C_{\max}$ ,  $C_b$  is either  $C_1$  or  $C_2$ , and the values of  $C_a$  and  $C_b$  are chosen to minimize the difference.

The formula for  $lt_{\text{eff}}$  outside the interval produces a graded mesh with an edge length that falls off parabolically with distance from the interval. Default values for the parameters of the interval refinements are defined in the Parameter Database (PDB).

## Summary of Refinement Parameters

**Table 86** lists `refinebox` parameters in the left column that can be used to specify boxwise refinement. The right column lists the corresponding PDB parameters that can be used to specify refinement criteria globally.

Table 86 Summary of refinement parameters

refinebox parameter	Corresponding entry in parameter database
<code>def.rel.error, rel.error</code>	Grid <Field> Refine.Rel.Error
<code>def.abs.error, abs.error</code>	Grid <Field> Refine.Abs.Error
<code>def.max.difference, max.difference</code>	Grid <Field> Refine.Max.Difference
<code>def.max.logdiff, max.logdiff</code>	Grid <Field> Refine.Max.LogDiff
<code>def.max.asinhdiff, max.asinhdiff</code>	Grid <Field> Refine.Max.AsinhDiff
<code>def.max.gradient, max.gradient</code>	Grid <Field> Refine.Max.Gradient
<code>def.max.dose.error, max.dose.error</code>	Grid <Field> Refine.Max.DoseError
<code>min.value</code>	Grid <Field> Refine.Min.Value
<code>max.value</code>	Grid <Field> Refine.Max.Value
<code>target.length</code>	Grid <Field> Target.Length
<code>target.length.scaling</code>	Grid <Field> Target.Length.Scaling

---

## Localizing Adaptive Meshing Using `refinebox` Command

Adaptive meshing has been implemented through generalized refinement boxes. As such, adaptive refinement and the refinement parameters themselves can be set in a boxwise manner. The default adaptive refinement box covers the entire structure and relies on global parameters and field-based parameters for its default values. If you specify an adaptive refinement box, the default box is not created.

**NOTE** For field-based refinement, any adaptive `refinebox` that is manually created overrides the default adaptive `refinebox`. The default adaptive `refinebox` (that covers the entire structure) can be created explicitly with the `refinebox adaptive` command.

You can create one or more adaptive refinement boxes with different parameters. The most commonly used parameters control the size of the box (`min` and `max`), and the minimum and maximum edge lengths (`refine.min.edge` and `refine.max.edge`).

The default list of fields upon which to refine includes all dopants, point defects, and clusters in the structure. This list can be modified in several ways. For example, the following command overrides the default list:

```
pdbSet Grid <field> DoNotAdapt 1
```

The next example adds `Field1` and `Field2` to the default list for this particular box:

```
refinebox refine.add.fields= { Field1 Field2 ... }
```

The following command redefines the list of fields to be used as the basis for refinement; if set, this command overrides any add or subtract settings for this particular box:

```
refinebox refine.fields= { Field1 Field2 ... }
```

## Examples

To switch on adaptive meshing, use:

```
pdbSet Grid Adaptive 1
```

To apply adaptive meshing only inside a box and to set the anisotropic edge minimum in the same box, use:

```
refinebox min= {0.0 0.0} max= {0.01 0.5} refine.min.edge= {0.001 0.25} adaptive
```

To refine only considering arsenic and boron, use:

```
refinebox refine.fields= {Arsenic Boron} adaptive
```

To create a default box and, in addition, to create a refinement box where  $r_F$  is modified locally for all species and  $\alpha_F$  is modified for only boron, use:

```
refinebox adaptive
refinebox min= {0.0 0.0} max= {0.01 0.5} def.rel.error= 0.9 \
abs.error= {Boron= 1.0e14} adaptive
```

## Adaptive Meshing During Diffusion

Adaptive meshing during diffusion is switched on by default when adaptive meshing is switched on (in other words, `pdbGet Grid Adaptive` returns 1). An additional control that prevents adaptive meshing at low temperatures is specified as:

```
pdbSet Grid Min.Adaptive.Temp <Temp C>
```

In any case, by default, adaptive meshing is not performed during oxidation or silicidation. You can switch on adaptive meshing during these steps by setting:

```
pdbSet Diffuse Compute.Regrid.Steps <n> ;# during inert annealings
pdbSet Diffuse Growth.Regrid.Steps <n> ;# during oxidation and silicidation
pdbSet Diffuse Epi.Regrid.Steps <n> ;# during epitaxy
```

where `<n>` is the fixed interval of time steps. For the parameter `Compute.Regrid.Steps`, the default is 10 steps and, for the other two parameters, the default is -1, meaning they are switched off by default. After the specified number of steps, the mesh is checked to decide whether the refinement criteria are satisfied (within some tolerance). A remesh is performed if necessary.

The refinement criteria check is performed as follows: Axis-aligned edges are checked to see whether they satisfy:

$$\text{actual} < \text{Refine.Factor} * \text{error} / \text{maxerror} \quad (991)$$

where:

- `Refine.Factor` is a direction-dependent parameter of the PDB under `Grid`.
- `error` is the error functions given in [Eq. 982–Eq. 987](#).
- `maxerror` is the maximum error parameter associated with each refinement type.
- `actual` is the ‘actual’ edge length.

## 11: Mesh Generation

### Adaptive Mesh Refinement

The parameter `Grid Refine.Percent` limits the percentage of edges that fail ([Eq. 991](#)) before a remesh is called. This check procedure is performed for every `Diffuse Compute.Regrid.Steps` whether a remesh is called or not. You can omit the refinement criteria check (which can be time-consuming for large meshes) and force a remesh by setting:

```
pdbSet Grid Refine.Check 0
```

[Table 87](#) summarizes the parameters available for adaptive meshing for diffusion.

Table 87 Adaptive meshing parameters for diffusion

Parameter	Description
<code>Compute Compute.Regrid.Steps</code>	Number of diffusion steps before refinement criteria are checked to determine whether remeshing is required.
<code>Compute Pre.Regrid.Save</code>	To help with tailoring the mesh, files can be saved immediately before adaptive remeshing occurs during diffusion. The files are named <code>&lt;input_file_stub&gt;_preregrid_###_fps.tdr</code> where <code>&lt;input_file_stub&gt;</code> would be, for example <code>n1</code> , if the input file was <code>n1_fps.cmd</code> and <code>###</code> is an increasing index starting with 001.
<code>Grid Refine.Check</code>	If this parameter is set to 1 (true), refinement criteria are checked and remeshing occurs if necessary. If it is set to 0 (false), remeshing occurs without a check.
<code>Grid Refine.Factor</code>	Tolerance factor for marking an edge too long.
<code>Grid Refine.Percent</code>	Allowed percentage of edges that can be too long.

---

## Adaptive Meshing During Implantation

Adaptive meshing during implantation is active whenever adaptive meshing is switched on (in other words, `pdbGet Grid Adaptive` returns 1). It also can be enabled or disabled for each implantation step using the `Adaptive` option of the `implant` command.

Adaptive meshing during implantation differs from adaptive meshing for other process steps in one key respect: When performing an implantation step, the implanted concentrations are defined by analytic expressions instead of discretized field values. Therefore, the final values for the implanted fields are not known before the remeshing step begins, so they must be computed as the mesh is refined.

By default, refinement on damage is handled differently from refinement on dopants. For the analysis of damage, the gradient is usually uninteresting, but the location of the crystal–amorphous interface is often critical. Therefore, refinement must be added to the mesh according to whether the damage is near the amorphous–crystal threshold, not according to the damage gradient. This is accomplished using an interval refinement (see [Interval Refinement](#)

([Criteria on page 734](#)). By default, the minimum and maximum values of the interval are set to the value of the amorphous–crystal threshold ( $1.15 \times 10^{22} \text{ cm}^{-3}$ ). The target length is  $0.002 \mu\text{m}$ , and the target length scaling is 1.0.

**NOTE** The default target-length setting of 2 nm can produce many mesh points for amorphizing implantations in three dimensions. You should first try using a larger setting and then reduce it if necessary.

As the mesh is constructed, each cell of the refinement tree is evaluated to determine whether the refinement criteria are satisfied. The criteria for as-implanted fields are computed for each edge of the cell. If any criterion is not satisfied, the cell is split and the as-implanted concentrations are computed at the newly introduced points. This process continues until all refinement criteria are satisfied (or the minimum edge length is reached) for all cells on the refinement tree. Therefore, the constructed mesh satisfies the refinement criteria for all fields present in the structure, not solely the implanted fields.

For adaptive meshing during Monte Carlo implantation, the analytic module is used to compute refinement, the mesh is formed, and afterwards, the implantation profiles are computed with the Monte Carlo module.

---

## Tips for Adaptive Meshing

Some useful suggestions when using adaptive meshing are:

- When setting boxwise meshing criteria, remember that any global criteria you have specified still apply inside the box. This means you cannot use boxwise meshing criteria to establish less stringent meshing criteria (such as a larger relative error) inside a box because the more stringent global criteria still apply. If you want to use different criteria for different parts of the structure, set the global criteria to the least stringent criteria and use boxes for more stringent criteria.
- To switch on adaptive meshing and use all the defaults, all that is needed is `pdbSet Grid Adaptive 1`. The main parameter for adjusting the amount of refinement is `pdbSet Grid AdaptiveField Refine.Rel.Error`, which defaults to 1.5. In many cases, this does not refine sufficiently. Decreasing the value causes more refinement. The number of mesh points is sensitive to this value, and it is not generally recommended to use a value less than 0.25. This parameter generally meshes doping gradients well, but may leave the peaks too coarse. To refine the peaks, the best criterion to use is maximum dose error (`Grid AdaptiveField Max.Dose.Error`).
- To override the default refinement box used for field-based refinement (which covers the whole structure and applies to all solution variables), you need only to create an adaptive refinement box. To add criteria in addition to the default criteria, for example, to add finer criteria under the gate while preserving standard parameters elsewhere, you can create your own default refinement box.

## 11: Mesh Generation

### Default Refinement

For example:

```
refinebox adaptive  
refinebox min= {-0.01 -0.01} max= {0.15 0.05} adaptive def.rel.error= 0.75
```

- The default refinement setting for implantation damage can give too fine a mesh. Increase Grid AdaptiveField Refine.Target.Length from the default value of 0.002 to reduce refinement.

---

## Default Refinement

In two dimensions, by default, interface refinement is applied to any interface in which one of the neighboring bulk regions is of material Silicon, Polysilicon, or Oxide. In two dimensions, the minimum normal mesh spacing near the interface is taken from the PDB parameter SnMesh min.normal.size. In three dimensions, by default, interface refinement is applied only to interfaces where one of the neighboring bulk regions is Silicon, and the minimum normal mesh spacing is taken to be a constant value (0.05  $\mu\text{m}$ ) to prevent excessive mesh points that could result from the default value of the PDB parameter Grid SnMesh (0.0008  $\mu\text{m}$ ). For other interfaces, the min.normal.size criterion is not applied. To view currently defined refinement boxes (including default refinement boxes), use:

```
refinebox print
```

Additional interface refinement can be specified with the command:

```
refinebox interface.materials= {<material1> <material2> ...}
```

This command specifies refinement at all interfaces to both <material1> and <material2>.

```
refinebox interface.mat.pairs= {<material1> <material2>}
```

This command specifies interface refinement at all interfaces where one side of the interface is <material1> and the other side is <material2>.

The interfaces that are refined are the union of interface.materials (all interfaces touching materials in the list) and interface.mat.pairs (only refined on material pairs found in the list first and second, third and fourth, and so on).

The default min.normal.size for all interface refinement boxes including the default ones is taken from the pdb parameter Grid SnMesh min.normal.size. Similarly, the default value of normal.growth.ratio for all interface refinement boxes is taken from the pdb parameter Grid SnMesh normal.growth.ratio.2d in two dimensions and from Grid SnMesh normal.growth.ratio.3d in three dimensions.

To add an interface refinement, use the refinebox command.

To remove an existing interface refinement, first execute `refinebox clear`, and then start again.

## Examples

The interfaces to be refined are defined as follows:

```
# Change the default min.normal.size (in micrometers)
pdbSet Grid SnMesh min.normal.size 2.0e-3

# Now modify which materials to apply interface refinement
# refine at all interfaces to silicon and poly (use the global min.normal.size
# and normal.growth.ratio)
refinebox clear
refinebox interface.materials= {silicon poly}
```

The next example shows refinement only at the silicon–oxide and polysilicon–oxide interfaces, and specifies a local value for interface refinement parameters:

```
refinebox clear
refinebox min.normal.size= 0.005 normal.growth.ratio= 3 \
interface.mat.pairs= {Silicon Oxide PolySilicon Oxide}
```

## Manipulating Refinement Boxes: transform.refinement Command

Transformations can be performed on refinement boxes using the `transform.refinement` command (see [transform.refinement on page 1246](#)), which works like the `transform` command, except for refinement boxes.

The `transform.refinement` command accepts the following:

- Transformation can be either `cut`, `flip`, `reflect`, `rotate`, `stretch`, or `translate`.
- Arguments depend on the type of transformation.
- `name` – applies the transformation to a particular refinement box if specified or to all refinement boxes otherwise.
- `name.new` – specifies the name of the transformed refinement box.
- `keep.original` – specifies whether to retain the original refinement box. Specifying `keep.original` preserves the original refinement box and creates a new transformed one. Specifying `!keep.original` transforms the specified refinement box. This option is useful when you want to ‘copy and paste’ refinements by, for example, translating them to a different position while keeping the original in place.

## 11: Mesh Generation

### Settings for Sentaurus Mesh

For example, the following command creates a new refinement box called newRefBox, which is identical to refbox but is displaced 0.1  $\mu\text{m}$  in the x-direction:

```
transform.refinement name= "refbox" name.new= "newRefBox" \
translate= {0.1 0 0} keep.original
```

---

## Settings for Sentaurus Mesh

[Table 88](#) lists the parameters available for Sentaurus Mesh. To set the parameters, use:

```
pdbSet Grid SnMesh <Parameter> <value>
```

Table 88 Parameters available for Sentaurus Mesh

Parameter	Default	Description
AllowRegionMismatch	false	If this parameter is set to true, when Sentaurus Mesh checks whether the number of regions in the input boundary and the number of regions at the end of the meshing process are the same, if there is a difference between the numbers of regions, Sentaurus Mesh will ignore the discrepancy, and the meshing process will continue. If this parameter is set to true and MinimumRegionMismatchVolume has also been specified, Sentaurus Mesh checks the volumes of all deleted regions: <ul style="list-style-type: none"><li>• If the volume of a deleted region is <i>less than the value</i> specified by MinimumRegionMismatchVolume, the meshing process will continue and the number of deleted regions is reported.</li><li>• If the volume of a deleted region is <i>greater than the value</i> specified by MinimumRegionMismatchVolume, the meshing process will stop.</li></ul> By default (when this parameter is set to false), when Sentaurus Mesh checks whether the number of regions in the input boundary and the number of regions at the end of the meshing process are the same, if there is a difference between the numbers of regions, the meshing process will stop.
Apply.Brep.DelPSC	false	Indicates whether the Delaunay refinement for piecewise smooth complex (DelPSC) algorithm is applied to the boundary at the beginning of a mesh generation step. DelPSC multithreading is controlled by: math numThreadsSnMesh
Apply.Brep.DelPSC.Accuracy	1e-4 $\mu\text{m}$	Specifies the accuracy used by the DelPSC algorithm when approximating high-curvature areas. In general, setting this parameter to 2% of the radius of curvature is appropriate. Larger values allow the DelPSC algorithm to run faster but generate coarser discretization on curved surfaces. Smaller values make the DelPSC algorithm run slower and generate finer discretization on curved surfaces.

Table 88 Parameters available for Sentaurus Mesh

Parameter	Default	Description
Apply.Brep.DelPSC.Resolution	1e-2 $\mu\text{m}$	Controls the size of small triangles in the DelPSC algorithm. In general, setting this parameter to 10% of the radius of curvature is appropriate. Larger values allow the DelPSC algorithm to run faster but generate bigger triangles next to geometric features and triple lines on curved surfaces. Smaller values make the DelPSC algorithm run slower and generate smaller triangles next to geometric features and triple lines on curved surfaces.
Apply.Brep.DelPSC.Ridge.Angle	150 degrees	Angle threshold to detect geometric features.
binarytree.split.box		Specifies the region where the binary-tree split factors are applied. In two dimensions: pdbSet Grid SnMesh binarytree.split.box \ {xmin 0.0 ymin 0.0 xmax 1.0 ymax 1.0} In three dimensions: pdbSet Grid SnMesh binarytree.split.box \ {xmin 0.0 ymin 0.0 zmin 0.0 xmax 1.0 ymax 1.0 \ zmax 1.0}
binarytree.split.factor.x	1	Splits the final binary tree used for refinement by the specified factor in the x-direction. Powers of 2 must be used.
binarytree.split.factor.y	1	Same as <code>binarytree.split.factor.x</code> but for the y-direction.
binarytree.split.factor.z	1	Same as <code>binarytree.split.factor.x</code> but for the z-direction.
CoplanarityAngle	175 degrees	Any pair of faces with an angle of <code>CoplanarityAngle</code> or more will be considered coplanar.
CoplanarityDistance	1.0e-6 $\mu\text{m}$	Maximum deformation caused to the boundary when swapping the edge shared by a pair of adjacent faces.
DecimateBeforeImprint	true	Decimates the boundary before imprinting it with the axis-aligned mesh.
DelaunayTolerance	1.0e-4	Specifies how close the ridges and boundary faces conform to the Delaunay criterion.
DelaunayToleranceMat		Specifies an array pair of materials and tolerances to be used in those materials. For example: pdbSet Grid SnMesh DelaunayToleranceMat {Silicon 0.01 Oxide 1.0}
DelaunayToleranceReg		Specifies an array pair of regions and tolerances to be used in those regions.
DelaunayType	conformal	Types of mesh generated by Sentaurus Mesh. Available types are box method, conformal, or constrained.

## 11: Mesh Generation

### Settings for Sentaurus Mesh

Table 88 Parameters available for Sentaurus Mesh

Parameter	Default	Description
DelPsc	false	Indicates whether the Delaunay refinement for piecewise smooth complex (DelPSC) algorithm is applied to the boundary at the beginning of a mesh generation step.
DelPscAccuracy	1e-4 $\mu\text{m}$	Specifies the accuracy used by the DelPSC algorithm when approximating high-curvature areas. This parameter is used during standard mesh generation (as opposed to using DelPSC during oxidation).
EdgeProximity	0.05	Specifies the minimum ratio of the edges generated when an edge is split.
FaceProximity	0.05	Specifies the minimum ratio of the faces generated when a face is split.
ImprintAccuracy	1e-5 $\mu\text{m}$	Distance used to determine when two points are too close during imprinting.
ImprintCoplanarFacesOnly	true	Imprints the binary tree on the coplanar sets of faces. This is useful to avoid over-refinement in curved areas.
ImprintCoplanarityAngle	179 degrees	Angle used to decide when two faces are coplanar. If two adjacent faces have an angle greater than this value, they will be added to the set of faces to be imprinted with the binary refinement tree cells.
ImprintCoplanarityDistance	1e-4 $\mu\text{m}$	Distance used to determine when two faces are coplanar. If the distance from one face to the plane of the other face is less than this value, they will be added to the set of faces to be imprinted with the binary refinement tree cells.
max.box.angle.2d	120 degrees	Maximum angle in binary tree (2D only).
max.box.angle.3d	150 degrees	Maximum angle in binary tree (3D only).
max.lateral.size	10 $\mu\text{m}$	Specifies the maximum lateral spacing between elements in the direction parallel to the interface.
MaxAspectRatio	1e6	Specifies the maximum-allowed aspect ratio of an element in the binary tree.
MaxBoundaryCutRatio.2d	0.01	Specifies the maximum-allowed ratio between the lengths of adjacent axis-aligned edges cutting material boundaries (2D only).
MaxBoundaryCutRatio.3d	0.01	Specifies the maximum-allowed ratio between the lengths of adjacent axis-aligned edges cutting material boundaries (3D only).
MaxConnectivity	1e37	Specifies the maximum number of elements connected to a point in the final mesh.

Table 88 Parameters available for Sentaurus Mesh

Parameter	Default	Description
MaxNeighborRatio	3.0	Binary-tree smoothing is performed after refinements have been added to the binary tree. This prevents sudden changes in the element size that can be especially detrimental to mechanics results. The ratio of neighboring collinear edges in the binary tree can be adjusted with this parameter.
MaxPoints	500000	Maximum number of points allowed by the Sentaurus Mesh delaunization module.
MaxSolidAngle	360 degrees	Specifies the maximum solid angle allowed in the elements of the mesh (3D only).
MaxTetQuality	1e37	Specifies the maximum circumscribed sphere radius-to-shortest edge ratio allowed in the mesh (3D only).
min.normal.size	8e-4 $\mu\text{m}$	Specifies the smallest normal (to the interface) mesh element size on either side of an interface.
MinAngle	0	Specifies the minimum angle allowed in the elements of the mesh (2D only).
minedge	2.0e-6 $\mu\text{m}$	Minimum edge length request.
MinimumRegionMismatchVolume	0	Specifies a region volume that Sentaurus Mesh uses when checking deleted regions. It is used in conjunction with AllowRegionMismatch set to true.
normal.growth.ratio.2d	2.0	Factor used to increase the size of the elements in the direction normal from the interface. The size of each layer equals the size of the previous layer multiplied by this factor (2D only).
normal.growth.ratio.3d	3.0	Factor used to increase the size of the elements in the direction normal from the interface. The size of each layer equals the size of the previous layer multiplied by this factor (3D only).
offsetting.maxlevel	3	Specifies the number of offsetting layers at an interface when Sentaurus Mesh offsetting is used at an interface.
SliverAngle	175 degrees	Limits the maximum dihedral angle on one element when the delaunizer performs the sliver removal step.
SliverDistance	1e-2 $\mu\text{m}$	Limits the amount of “damage” done to the standard Voronoï diagram by the sliver removal algorithm. Note that the grid produced by the sliver removal algorithm is weighted Delaunay, so the standard Voronoï diagram is “damaged” unless the Voronoï weights are stored (see the StoreDelaunayWeight parameter). When the box method library reads those weights, it calculates the correct Voronoï diagram and coefficients to solve the PDEs.
SliverRemovalAlgorithm	1	Algorithm for sliver removal, either 1 (original) or 2 (reduced non-Delaunay elements).

## 11: Mesh Generation

### Displaying Refinement Boxes

Table 88 Parameters available for Sentaurus Mesh

Parameter	Default	Description
StoreDelaunayWeight	0	When set to 1, stores the Delaunay–Voronoi weight ( <code>DelVorWeight</code> ) for the box method library.
UseLines	true	Specify 1 or 0. <code>UseLines</code> is specified in the <code>line</code> command in the mesh generated by Sentaurus Mesh.

## Displaying Refinement Boxes

Refinement boxes are saved to TDR files for displaying in Sentaurus Visual. When loading a TDR file in Sentaurus Visual, if refinement boxes are present, `RefinementBox` will be listed on the **Materials** tab (see [Figure 87 \(left\)](#)). The list of individual refinement boxes is found on the **Lines/Particles** tab (see [Figure 87 \(right\)](#)).

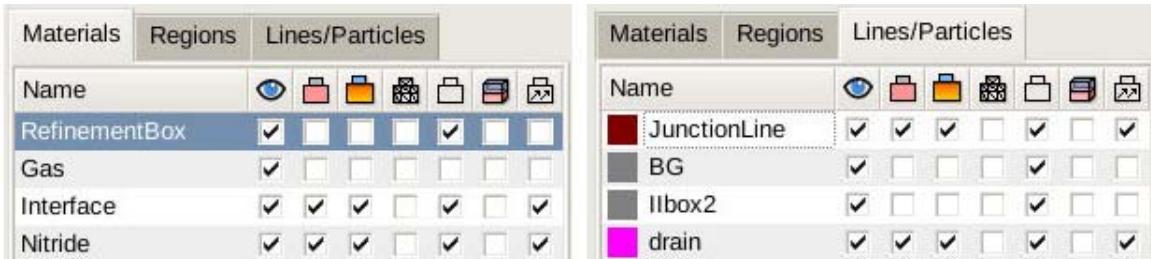


Figure 87 (Left) Materials tab showing `RefinementBox` and (right) Lines/Particles tab showing refinement boxes

By default, refinement boxes are not displayed. They may be displayed in bulk or with borders. [Figure 88 on page 747](#) shows a 2D structure with two refinement boxes and its corresponding mesh. [Figure 89 on page 747](#) shows a 3D structure with two refinement boxes and its corresponding mesh.

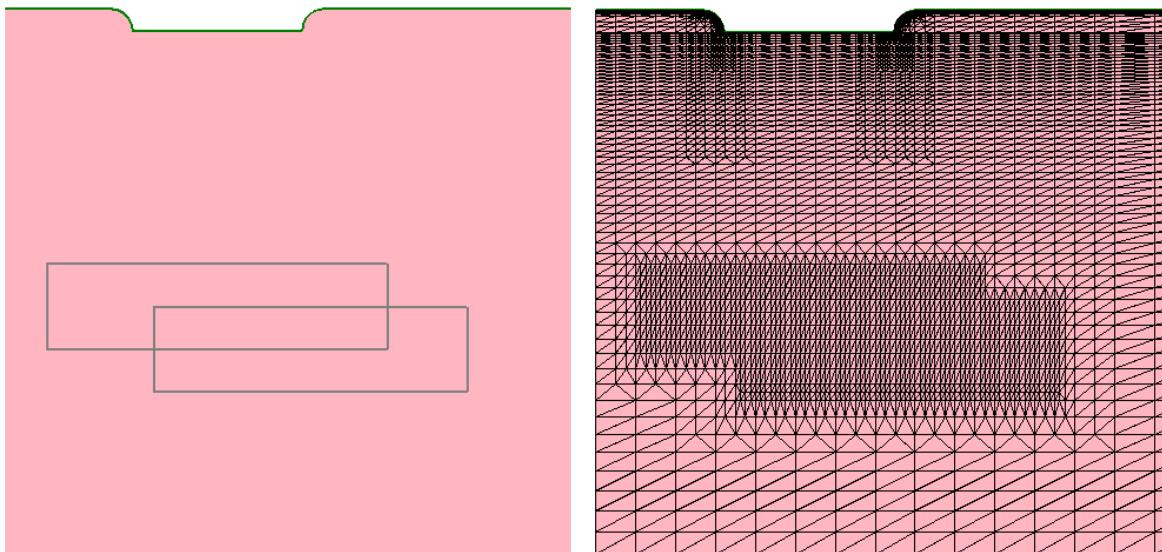


Figure 88 (Left) Two-dimensional structure with two refinement boxes and (right) corresponding mesh

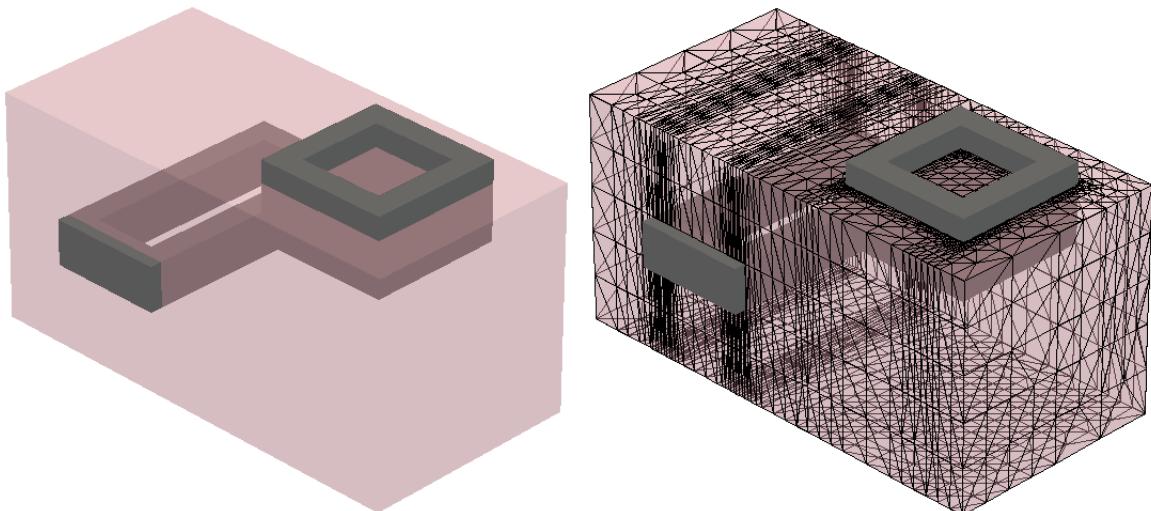


Figure 89 (Left) Three-dimensional structure with two refinement boxes and (right) corresponding mesh

## Controlling the Mesh During Moving-Boundary Problems

Moving-boundary problems create new regions and dramatically alter the shape of existing ones. Controlling the mesh is important. This section covers some mesh control methods.

---

### TSUPREM-4 Moving-Boundary Meshing Library

The TSUPREM-4 moving-boundary meshing library is available from within Sentaurus Process (hereafter, referred to as the *TS4 mesh library*). By default, the TS4 mesh library performs all mesh updates in 2D moving-boundary oxidation simulations.

The TS4 mesh library deposits the native oxide layer before oxidation by default. Since it removes all grids inside a gas region, the simulation performance is improved without any loss of accuracy.

For silicidation, a gas mesh is used by default. The following statement forces the use of a TSUPREM-4-style gas mesh instead of the default gas mesh:

```
pdbSet Grid UseTS4GasMesh 1
```

### Control Parameters in TS4 Mesh Library

The control parameters of the TS4 mesh library are specified with:

```
pdbSet Grid TS4Mesh <control parameter> <value>
```

The available control parameters are:

**MergeSubAndAdd <0 | 1> (default: 1)**

It optimizes the speed performance by merging the grid subtraction and addition procedures.

**DoSubAfterStep <0 | 1> (default: 0)**

Grid points that are too close to the moving boundary are removed after each diffusion step, while grid addition is performed after each mechanics step followed by the diffusion step. Switching on this flag forces only one diffusion step per each mechanics step. When this flag is switched on, MergeSubAndAdd is ignored.

**SubTimeFactor <double> (default: 1.5)**

The time step given by mechanics for grid removal is scaled by SubTimeFactor.

**NOTE** Do not change the default.

`MinSpaceOnInterface <double> (default: 2e-6 [ $\mu\text{m}$  ])`

The nodes on an interface mesh must be rebuilt after meshing on the moving boundary since the bulk meshes along the interface can be added or removed. Instead of destroying and rebuilding the interface mesh, the TS4 mesh library tries to reuse the original node data on the interface mesh to minimize the interpolation error. The original nodes are detected when the location difference is less than `MinSpaceOnInterface`.

**NOTE** Do not change the default.

`ExactGridSpace <0 | 1> (default: 1)`

On the growing material side of the interface, the triangular mesh elements expand. To maintain solution accuracy in the material (for example, calculating the diffusion of oxidant in the oxide), you must add nodes to the growing material. The addition of nodes to the growing material is controlled by `perp.add.dist`, `ExactGridSpace`, and `LocalGridSpace`.

**NOTE** `perp.add.dist` is the grid control parameter of each material, for example: `pdbSet Oxide Grid perp.add.dist 0.01e-4`

Precise grid spacing is obtained by adding new nodes in a growing layer at the distance specified by `perp.add.dist` from the existing node in the layer. Because only one node can be added at each point on an interface during a simulation time step, the size of the time step may need to be reduced to achieve the required spacing. This reduction in the time step size can be disabled by specifying:

`pdbSet Grid TS4Mesh ExactGridSpace 0`

By default, `ExactGridSpace` is set to 1 to allow reducing the size of the time steps to control the grid spacing. The algorithm does not allow grid points to be added at spacings less than 1 Å, and control of the spacing may not be precise for spacings less than 2 Å.

`LocalGridSpace <0 | 1> (default: 1)`

The grid control algorithms and parameters apply to the entire structure. To avoid adding a very fine grid in field regions when growing gate oxides, an option allows the grid spacing to vary with the oxide growth rate. When `LocalGridSpace` is switched on, the grid spacing to be used at each point in the growing material is:

$$h = (v_{\max}/v) \text{ perp.add.dist}$$

where  $v$  is the growth rate at a point in the structure, and  $v_{\max}$  is the maximum growth rate at all interfaces of the same type in the structure. `LocalGridSpace` is switched on by default.

## 11: Mesh Generation

### Controlling the Mesh During Moving-Boundary Problems

`OrderFlatTri <0 | 1> (default: 1)`

When the area of a shrinking triangle becomes less than  $1e-15$  ( $\text{cm}^2$ ) after a time step, the triangle is removed. When the shrinking triangle to be removed is located at a material interface and the removal of the triangle will result in a bad mesh, the material type of the shrinking triangle is replaced with the type of the growing neighbor material, instead of removing it. When those triangles are adjacent to each other, the reordering algorithm for the replacements smooths the interface shape after conversion.

`MinAreaRemovalRatio <double> (default: 10.0)`

When a region has only one triangle surrounded by neighbors of different materials and its area is less than `MinAreaRemovalRatio` multiplied by  $1e-15$  ( $\text{cm}^2$ ), the material type of the triangle is replaced with the neighbor material that shares the longest edge with the triangle.

`Min.Split.Distance <double> (default: 1e-8 [cm])`

When multiple regions with the same material meet at one point, the point is split by inserting new elements. The parameter determines the minimum split distance.

---

## Moving Mesh and Mechanics Displacements

The displacements computed by the mechanics solution during oxidation are applied to the nodes after checking against the `MinimumVelocity` criterion defined for each region. Velocity is the computed solution variable and is multiplied by the time step to compute displacements. The nodes are moved by this amount.

The computed velocities are compared against `MinimumVelocity` and, if the computed velocity is greater than `MinimumVelocity`, the displacements are computed and applied. The `MinimumVelocity` is set with the command:

`pdbSetDouble Silicon Grid MinimumVelocity <n>`

---

## Controlling the Grid Spacing

Grid spacing in the growing region is controlled by `perp.add.dist`. Its unit is centimeter, and the edges in growing regions are checked to see whether they are nearly perpendicular to the interface.

If they are perpendicular, they are split if their length exceeds the value of `perp.add.dist`. This value is set with the command:

`pdbSet Oxide Grid perp.add.dist 2e-7`

## Cleaning Up the Grid

During oxidation or silicidation, the growing region increases at the expense of a shrinking region. The shrinking regions then have a problem of small edges. Below a certain value, these edges must be removed entirely, and the mesh around them must be adjusted.

The short edge criterion is specified by the `Remove.Dist` parameter, which is specified in centimeters and is set as follows:

```
pdbSet Silicon Grid Remove.Dist 3e-8
```

**NOTE** Due to mesh quality constraints, this value must be more than  $2 \times 10^{-8}$  cm.

---

## Maximum-Allowed Rate of Growth

For a minimal simulation time, it would be best if the entire thickness growth were simulated in one step. However, this is not possible for different reasons, including:

- Nonconvergence of diffusion equations.
- Inability to track material interfaces if they grow more than one edge length of a triangle or a tetrahedron.

In the new growing region, new nodes are introduced and the data is interpolated from the nearby nodes. If growth is too fast, significant interpolation errors could occur.

The rate of growth can be controlled by the parameters `dThickness` and `IncreaseRatio`. The `dThickness` parameter (specified in micrometers) defines the maximum-allowed oxidation front displacement per time step and is set as follows:

```
pdbSet Diffuse dThickness 0.001
```

The `IncreaseRatio` parameter is the factor by which the time integration step is allowed to grow. The time integration step will increase until the resulting increase in film thickness exceeds the value allows by `dThickness`.

---

## Miscellaneous Tricks

Since Sentaurus Process oxidation does not allow the interface to traverse more than one element thickness at a time, speed can be achieved by having elements with longer edge lengths near the interface.

## 11: Mesh Generation

### Controlling the Mesh During Moving-Boundary Problems

This can be controlled by refinement boxes or the `pdb` parameter `Grid SnMesh min.normal.size`. Large structures, like those used in power devices, may need `min.normal.size` of 0.01  $\mu\text{m}$ , while submicron CMOS devices need 8 Å.

The parameter `Grid SnMesh normal.growth.ratio.3d` controls the mesh away from the interface. If the mesh spacing does not increase fast enough, this number can be increased.

In large structures, the interface fidelity may not need to be as tight as that of 45-nm or 32-nm gate transistors. The `accuracy` argument of the `mgoals` command can be increased to 1 Å (`mgoals accuracy= 1e-4`), which will cause MGOALS to clean up interfaces of small (sub-1 Å) features and ensure smooth long edges that speed up oxidation.

These are options available to the simulation engineer; however, care must be exercised in varying these parameters since they may affect the final structure significantly.

---

## Meshing for 3D Moving-Boundary Problems

Maintaining a conformal high-quality mesh during the simulation of a 3D moving mesh is very difficult because of the following requirements: moving boundaries, accurate profiles, dose conservation, minimization of the number of mesh points, and maintaining high-quality mesh elements. In particular, handling the frequent collision of the moving front with points inside the other regions can cause intractable problems for the local mesh operations needed for maintaining dose conservation.

Before each time-step, the mesh is checked for the maximum-possible time step until the first tetrahedral element collapses (becomes flat) in the material being consumed (that is, silicon). If necessary, the time step is reduced. During simulation, all mesh points are moved using the velocity and the time step. The mesh topology is not changed during the solve time step. At the end of the solve time step, the mesh quality is improved and flat elements are removed, allowing the next time step to be sufficiently large.

---

## MovingMesh Algorithm

**NOTE** The MovingMesh algorithm is experimental and requires careful parameter settings. Contact TCAD Support for technical assistance.

The MovingMesh algorithm is used for 3D moving-boundary problems such as oxidation and silicidation. It can be switched on and off with the following command before a diffuse command:

```
pdbSet Grid Use.MovingMesh 1      ;# switched on by default
```

Three important parameters control MovingMesh:

```

pdbSet Oxide Grid perp.add.dist 0.005e-4      ;# centimeter
pdbSet Grid Remove.Dist 0.001e-4              ;# centimeter
pdbSet Grid MovingMesh Remove.Dist.On.Interface 0.0001e-4 ;# centimeter

```

The `perp.add.dist` parameter specifies the distance (in cm) that the oxide interface can move before new mesh points are inserted in the oxide.

The `Remove.Dist` parameter specifies the shortest distance (in cm) the mesh vertices are allowed from the interface into the bulk. For lengths shorter than this distance, the vertices will be removed. Do not specify a distance larger than the minimum material thickness, which is typically the thickness of the native layer. For a typical example with 1.5 nm native layer, `Remove.Dist` of 1.0 nm or less is appropriate.

The `Remove.Dist.On.Interface` parameter controls small triangles on material interfaces. Triangles with an edge shorter than this distance will be removed. A smaller number makes the interfaces smoother, but results in a larger number of triangles.

The oxide interfaces can develop problematic geometric features such as knife edges, noisy surfaces, or extremely thin gaps. You can enable geometry repair and surface remeshing by using:

```

pdbSet Grid MovingMesh Repair.Geometry 1      ;# switched on by default

```

The criteria to trigger geometry repair are based on the minimum dihedral angle and the maximum face angle:

```

pdbSet Grid MovingMesh Repair.Geometry.Min.Dihedral.Angle 5 ;# degree
pdbSet Grid MovingMesh Repair.Geometry.Max.Face.Angle 175 ;# degree

```

If the minimum dihedral angle between two triangles is below the threshold or the maximum face angle of a triangle is above the threshold, the geometry repair procedure starts.

The geometry repair procedure involves a multimaterial level-set (MLS) formulation. The resolution of the level-set cell size is controlled by:

```

pdbSet Grid MovingMesh Repair.Geometry.Resolution 0.001 ;# micrometer

```

**NOTE** The parameter `Repair.Geometry.Resolution` must be, at most, one-third the thickness of the thinnest region. Otherwise, the thin region may be considered noise, and it disappears.

## 11: Mesh Generation

### Controlling the Mesh During Moving-Boundary Problems

**NOTE** The amount of geometry smoothing performed by the MLS algorithm depends on both the curvatures in the input and the level-set cell size. A noisy surface has a high curvature, so it will be smoothed to a large extent to remove noise. On the other hand, a planar surface has zero curvature and is well preserved. Unfortunately, a sharp corner has a theoretically infinite curvature, so it will become a rounded corner. When the corner is rounded, the next iteration of MLS smoothing will have less effect. The specified level-set cell size is the threshold to distinguish between the noise to be removed and the features to be preserved.

The boundary representation (brep) of the new geometry must go through a meshing algorithm for curved surfaces called the Delaunay refinement for piecewise smooth complex (DelPSC) that improves the quality of triangles on brep surfaces. This algorithm is enabled by:

```
pdbSet Grid MovingMesh Apply.Brep.DelPSC 1      ;# switched on by default
```

The DelPSC algorithm performs adaptive sampling on ridges (1D geometric feature) according to the refinement fields, the curvatures of the ridges, and the proximity among the ridges. On each surface patch (2D geometric feature), the DelPSC algorithm performs adaptive sampling according to the refinement fields and the curvatures of the surface. Multithreading in the DelPSC algorithm is controlled by `math numThreadsSnMesh`.

Ridge sampling also is controlled by:

```
pdbSet Grid MovingMesh Apply.Brep.DelPSC.Resolution 0.005    ;# micrometer
```

The above parameter ensures no ridge edge will be longer than the specification. It is useful, for example, when you have a straight line (no curvature) next to curved surfaces. You want the sampling points on the straight line to be fine enough to support the adjacent curved surfaces.

Note that you no longer require `Apply.Brep.DelPSC.Resolution` to be as small as the thin native layer thickness, because of the adaptive sampling based on proximity between nearby ridges.

To control accuracy in high curvature areas, you can specify the acceptable distance between the old and new curved surfaces using:

```
pdbSet Grid MovingMesh Apply.Brep.DelPSC.Accuracy 0.0001    ;# micrometer
```

**NOTE** Every time the DelPSC algorithm is applied, the new curved surface can deviate from the old curved surface by, at most, the value of `Apply.Brep.DelPSC.Accuracy`. New vertices lie exactly on the old surface, but new triangles cannot lie exactly on the old surface *unless* the old surface is flat. In general, the smaller the value of `Apply.Brep.DelPSC.Accuracy` is, the smoother the new surface

becomes, and the more accurate the new surface represents the old surface.

These are typical settings for a small transistor structure:

```

pdbSet Oxide Grid perp.add.dist 2e-7          ;# cm 2nm
pdbSet Silicon Grid perp.add.dist 1e-6         ;# cm 10nm
pdbSet Grid Remove.Dist 9e-8                  ;# cm 9A
pdbSet Grid MovingMesh Remove.Dist.On.Interface 3e-8 ;# cm 3A
pdbSet Grid MovingMesh Repair.Geometry.Resolution 3e-4 ;# um 3A
pdbSet Grid MovingMesh Apply.Brep.DelPSC.Resolution 3e-3 ;# um 3nm
pdbSet Grid MovingMesh Apply.Brep.DelPSC.Accuracy 1e-4 ;# um 1A

```

These are typical settings for a large power structure.

```

pdbSet Oxide Grid perp.add.dist 2e-6          ;# cm 20nm
pdbSet Silicon Grid perp.add.dist 1e-5         ;# cm 100nm
pdbSet Grid Remove.Dist 9e-7                 ;# cm 9nm
pdbSet Grid MovingMesh Remove.Dist.On.Interface 3e-7 ;# cm 3nm
pdbSet Grid MovingMesh Repair.Geometry.Resolution 3e-3 ;# um 3nm
pdbSet Grid MovingMesh Apply.Brep.DelPSC.Resolution 3e-2 ;# um 30nm
pdbSet Grid MovingMesh Apply.Brep.DelPSC.Accuracy 1e-3 ;# um 1nm

```

MovingMesh has facilities for troubleshooting runtime failures. A typical setting would be:

```

# Switch on level-1 diagnostics
pdbSetDouble debugLevel MovingMesh 1           ;# switched off by default

# Save intermediate result every 100 time steps
pdbSetDouble Grid MovingMesh Save.Interval 100 ;# switched off by default

# Save diagnostic files for Repair.Geometry and DelPSC
pdbSetBoolean Grid MovingMesh Repair.Geometry.Monitor 1
                                              ;# switched off by default

```

In level-1 diagnostics, the intermediate result will be saved after a certain number of time steps in the files:

<NodeName>\_MovingMeshGridTimeStep<xxxx>.tdr

The frequency of saving is specified by the `Save.Interval` parameter. The files are written after mechanics and before diffusion to analyze the grid-limited time step.

In the event of failure in `Repair.Geometry`, the level-1 diagnostics will save files with names such as:

```

<NodeName>_remeshBrep{In,MLS,PSC,Out}.tdr
<NodeName>_applyBrepDelPSC{In,Out}.tdr

```

## 11: Mesh Generation

### UseLines: Keeping User-Defined Mesh Lines

They are useful for checking whether the resolution parameters are adequate. The most likely cause of failure is a too coarse resolution to capture thin oxide layers and other small geometric features.

If the parameter `Repair.Geometry.Monitor` is set to 1, the intermediate files with names such as:

```
<NodeName>_remeshBrep_<xxxx>_{In,MLS,PSC,Out}.tdr  
<NodeName>_applyBrepDelPSC_<xxxx>_{In,Out}.tdr
```

will be saved every time the repair geometry operation is triggered. These files are useful to monitor how the MLS and DelPSC algorithms perform at various points in a simulation.

---

## UseLines: Keeping User-Defined Mesh Lines

During the `init` command, the line location and spacing specifications given by `line` commands are expanded into ticks and stored in the PDB and in TDR files. This is performed by default.

By carefully placing lines, you can isolate areas of the structure that changed (because of etching, deposition, and so on) from those that do not (such as bulk silicon). In this way, the mesh in areas that do not change will have the least amount of change, the least interpolation, and the most accurate results. Even the mesh in regions that do change will have a similar starting point and should also have minimal mesh-point movement coming from remeshing.

Lines for Sentaurus Process Kinetic Monte Carlo are stored separately from the lines used with continuum solvers (in other words, Sentaurus Mesh meshes). By default, `line` commands are applied to both kinetic Monte Carlo and continuum meshes. Use `!kmc` or `!mgoals` to not apply a particular `line` command. For example, for a `line` command to apply only to continuum meshes, use `line !kmc`.

In the simplest case, all the `line` commands are specified before the `init` command, and they are saved and reused every time a remesh is performed. However, there are other cases described in the following sections that allow this feature to be more powerful.

---

## Using line Commands After init Command

The expansion of lines from `line` commands into ticks (in other words, all starting mesh line locations) is performed only at the point that the lines in that direction are needed. For example, x-lines are always expanded in the `init` command, but y-lines are only expanded when the first etch with a mask is given. Therefore, it is possible to load a 1D structure, give y-lines, and then expand to 2D, or give both y- and z-lines and expand to 3D.

After a particular direction or dimension is expanded, it is only possible to insert one tick at a time in that direction using the `line` command (in other words, the `spacing` parameter is thereafter ignored). For example, inserting additional lines in this matter could be useful because you identified the amorphous–crystalline interface in silicon.

This is handled by specifying one of the following:

- The `line` command in a dimension greater than the current dimension. For example, a y-line specification when the simulation is one dimensional.
- The `line` command in a dimension at or less than the current dimension. For example, either an x-line or a y-line specified when the simulation is two dimensional.

For more information, see [Automatic Dimension Control on page 42](#).

## Dimension Within Current Spatial Dimension

This is encountered if the user-specified x-lines and the current spatial dimension of analyses is 1D. Or, it could happen if you specify x- or y-lines in 2D, or x-, y-, or z- lines in 3D.

In this case, the `line` command ignores the `spacing` parameter and tries to insert only one tick as long as that tick (line) is not too close to an existing tick.

Inside the `init` command, the `line` commands are expanded into ticks using the `spacing` specifications for the dimension as they are needed. When additional `line` commands are given for dimensions where the ticks have already been expanded, the `spacing` parameter is ignored and one additional tick is added as long as it is not too close to an existing tick.

## Dimension Greater Than Current Spatial Dimension

This is encountered if you specified y- or z-lines, and the current spatial dimension of analyses is 1D. Or, it could happen if you specify z-lines and the current spatial dimension of analyses is 2D.

In this case, the `line` command is considered in its entirety, and the `spacing` parameter is used. All the intermediate lines are included in the list of ticks kept.

---

## Using `line` Commands to Create Virtual Spacing

By default, the ticks created by the `line` command with the `spacing` argument are *hard* lines that Sentaurus Mesh enforces whenever possible. Since such lines traverse the entire structure, they can result in unnecessary refinement, especially if the `spacing` argument is used with small values.

## 11: Mesh Generation

### UseLines: Keeping User-Defined Mesh Lines

Using the `virtual.spacing` option, the ticks created between `line` commands become *soft* lines. This means that the refinement lines created by Sentaurus Mesh, during the binary tree construction, will snap to these ticks, thereby building a more predictable pattern instead of the pattern generated by the default bisection algorithm.

For example, the following commands create a virtual spacing of 1 nm on the device between the `(0, 0)` and `(1, 1)` coordinates. All user-defined refinement will snap to the coordinates defined in this virtual grid:

```
line virtual.spacing  
line x loc=0 spacing=0.001  
line x loc=1 spacing=0.001  
line y loc=0 spacing=0.001  
line y loc=1 spacing=0.001
```

**NOTE** The `virtual.spacing` option is applied globally and affects all lines at the same time.

---

## UseLines and the transform Command

The ticks must be handled in a special manner with the `transform` command (see [transform on page 1236](#)).

### Reflection

Using `transform reflect`, in the reflected region, the ticks are created after applying lateral inversion along the appropriate plane.

### Stretch

On applying `transform stretch` at a given coordinate in a given direction, the existing ticks in the stretched area are translated by the amount of the stretch. You must insert lines in the stretched area appropriately.

### Rotation

When applying `transform rotate`, the ticks also are rotated and properly transferred between x-ticks, y-ticks, and z-ticks.

## Translation

The `transform translate` command shifts the ticks by the specified amount.

## Cut

Using `transform cut`, the lines in the part of the structure that is cut are deleted.

---

## Example: Testing line Commands

Use the following example to test line commands:

```
line x loc=0 tag=a spacing=0.05
line x loc=0.1 spacing=0.05
line x loc=1 tag=b spacing=0.05
line y loc=0 tag=c spacing=0.01
line y loc=0.6 tag=d spacing=0.1

region silicon xlo=a xhi=b ylo=c yhi=d
init !DelayFullD

deposit oxide thickness=0.002 iso
grid remesh info=2

line y loc=0.026
line y loc=0.027
line y loc=0.028
line y loc=0.029
line y loc=0.025
line y loc=0.024
line y loc=0.023

grid remesh

deposit poly thickness=0.18 iso
mask name=m1 left=-0.1 right=0.025
etch aniso thickness=0.2 poly mask=m1

struct tdr=linetest
```

---

## Example: Showing Clearing Lines for a New Structure

Use the following example to show clearing lines and to prepare for another structure definition within the same command file:

```
line x loc=0 tag=a spa=0.125
line x loc=1 tag=b spa=0.125
line y loc=0 tag=c spa=0.125
line y loc=1 tag=d spa=0.125
region silicon xlo=a xhi=b ylo=c yhi=d
init

grid FullD

line clear

line x loc=0 tag=a spa=0.125
line x loc=1 tag=b spa=0.125
line y loc=0 tag=c spa=0.125
line y loc=1 tag=d spa=0.125
region silicon xlo=a xhi=b ylo=c yhi=d
init

line y loc=0.3 spa=0.01

grid FullD
```

---

## Data Interpolation

Sentaurus Process stores a copy of the mesh with all its data before performing any geometry-changing operation. This is the reference mesh used to interpolate data onto the new mesh. In three dimensions, a mesh is generated only when it is necessary, so you can have multiple `etch`, `deposit`, `photo`, and `strip` commands without the need to remesh in between. When a new mesh is required, data is interpolated from the stored mesh and data.

Data interpolation is performed materialwise. This is important because some nodal data can be discontinuous at material interfaces; for example, segregation causes a jump in concentration at the silicon–oxide interface. In addition, the precise location of an interface can change slightly due to numeric noise in geometry-moving algorithms. Therefore, it is necessary to allow the data to be interpolated from points in the old mesh nearby, but only from the same material.

Data also can be interpolated from materials that are *Like* materials (that is, the material in the old mesh is *Like* the material in the new mesh, or the material in the new mesh is *Like* the material in the old mesh). When interpolating data at an interface, the preference is to use data

from the same region, then data from the same material, and finally data from *Like* materials. If no match is found, then 0 is set for all data at that point.

For data defined on elements, the overlap of elements from the old mesh to the new mesh is used for weighting. Similar to nodal data, interpolation of elements near interfaces uses the region, material, and *Like* material preference order.

Multithreaded interpolation can be used to speed up interpolation in large 3D structures. Because of the memory-intensive nature of interpolation, the performance benefit of multithreading may saturate, but it depends strongly on the example. If the performance degrades when using a large number of threads, the following command can be used to reduce the number of threads for interpolation:

```
math numThreadsInterp=<i>
```

---

## Data Interpolation Near Boundaries

Region boundaries in a mesh can move for various reasons, including:

1. Geometric changes such as etching or deposition.
2. Boundary cleanup operations designed to reduce the number of boundary points and, therefore, the overall number of mesh points.
3. Moving-boundary simulations such as oxidation, silicidation, and model 0 type epitaxy.

The interpolation module has no information about all the operations that may have occurred since the last bulk mesh was created. Therefore, a tolerance is used to distinguish between boundary points displaced by case (1) where the boundary is expected to move more than a small amount, so interpolated values should be taken from exact locations in the new mesh, and cases (2) and (3) where the boundary should move only a small amount, so the values at the boundary should be transferred by interpolating from the nearest location on the old boundary.

The tolerance is set with the following command, where the distance is measured in micrometers:

```
pdbSet Grid Interpolation.Search.Distance <n>
```

## 11: Mesh Generation

### Troubleshooting

Figure 90 illustrates the meaning of this parameter.

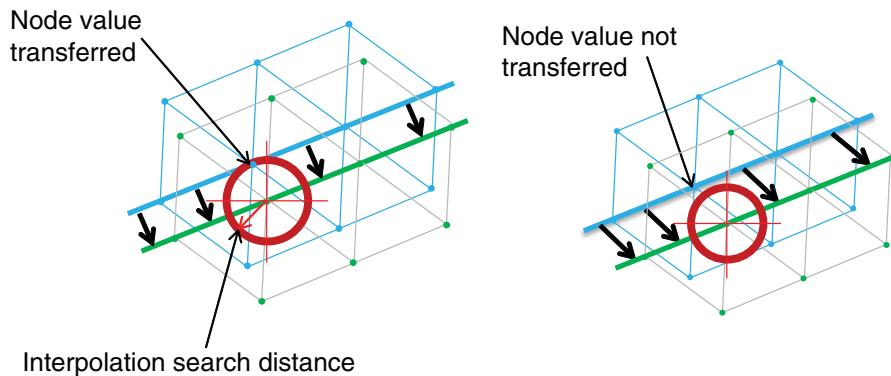


Figure 90 (Left) The new mesh (blue) has moved from its previous position, but the distance is smaller than Interpolation.Search.Distance, so values are interpolated from the green mesh to the blue mesh at the boundary. (Right) The distance is too large, so only those points in the blue mesh that are the same material as the green mesh are interpolated.

---

## Troubleshooting

Sometimes, the mesh generation step fails and it is unclear what the problem could be. The following are recommendations of where to look when problems arise during meshing:

- Set InfoDefault to 2 or higher, for example:

```
pdbSet InfoDefault 2
```

- When Sentaurus Mesh prints the message:

```
"Short edge 1e-8 around points (x1, y1, z1) (x2, y2, z2)"
```

look at the input structure around the coordinates  $(x_1, y_1, z_1)$  or  $(x_2, y_2, z_2)$ , and check whether there is a singularity in that area (such as a crack, fold, or surface overlap).

Sometimes, these singularities are the product of an etching or a deposition step, and action can be taken to improve the quality of the structure.

- Check the quality of the boundary printed for the steps preceding the mesh generation process. In particular, the following line provides an indication of quality (this is output if InfoDefault is 2 or higher):

```
minDihedralAngle: <angle> [near (x1, y1, z1), (x2, y2, z2)] at  
region=Nitride_1.
```

If you see an angle less than  $3^\circ$  in the geometry, this might indicate a problem in the structure at the given coordinates. Look at the preceding process steps in Sentaurus Visual to see whether they can be modified to avoid creating the problem.

To visualize the problem area in Sentaurus Visual, choose **View > Camera Configuration** to open the Camera Properties panel. On the panel, click the **Rotation Point** tab, enter one of the coordinates where the small dihedral angle is reported, and select the **Show** option under Point/Line. This will display a red 3D crosshair marker indicating the location of the center of rotation. You can hide all regions, except the one where the minimum dihedral angle is reported and zoom in around the red marker to locate the problem area. Sometimes you need to rotate the structure around the red marker to see what is happening to the geometry.

- You might need to add `!repair` to the `etch` or `deposit` command to ensure the structure is not repaired. This makes it easier to find the problem in Sentaurus Visual.
- Frequently save snapshots of the boundary file of the structure, especially before all mesh generation operations. This will help you to investigate possible problems in the input to the mesh generator. To accomplish this, use the command:

```
struct tdr.bnd=<c>
```

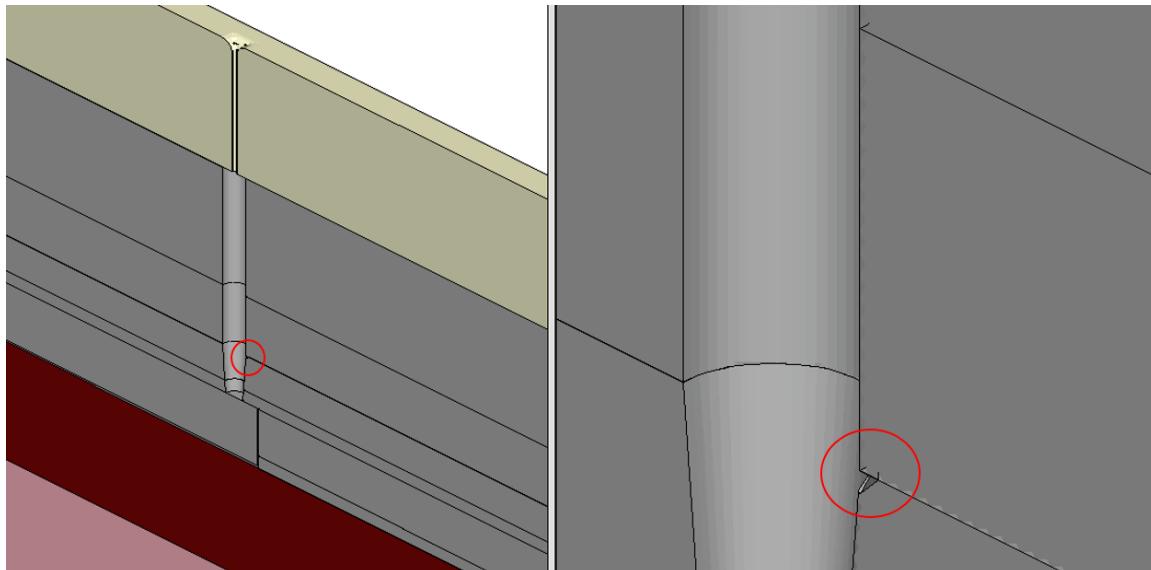


Figure 91 (Left) Example of artifact in geometry and (right) magnification of artifact (circled region)

## **11: Mesh Generation**

### Troubleshooting

# CHAPTER 12 Structure Generation

---

*This chapter describes etching, deposition, insertion, and other geometric transformations available in Sentaurus Process.*

## Overview

During device fabrication, several etching and deposition steps are necessary. Such steps can be modeled in Sentaurus Process by simple geometric operations or simple mathematical formulations in which no physical processing is simulated.

The creation of complex 3D shapes can be assisted by an interface to Sentaurus Structure Editor (see [Sentaurus Structure Editor Interface on page 829](#)) or the insertion of predefined pieces of a structure (see [Inserting Polygons on page 825](#) and [Inserting Polyhedra on page 826](#)). A shape library is available for commonly used structures (such as shallow trench isolation). These shapes are already parameterized (see [Shape Library on page 794](#)).

For physical etching and deposition, Sentaurus Process provides interfaces to Sentaurus Topography and Sentaurus Topography 3D (see [Sentaurus Topography Interface on page 832](#) and [Sentaurus Topography 3D Interface on page 834](#)).

Sentaurus Process provides several etching and deposition operations, in addition to purely geometric operations to help shape the geometry of devices:

- Etching is described in [Etching on page 766](#).
- Deposition is described in [Deposition on page 785](#).
- Masks offer an effect (similar to a masking layer) to limit the etching or deposition process to a certain window or to provide a convenient way to mimic lithographic patterning (see [Masks and Lithographic Patterning on page 802](#)).
- Several geometric transformations are available (see [Geometric Transformations on page 810](#)).
- The internal module, MGOALS, which is used to perform geometric etching and deposition, is described in [MGOALS on page 816](#).

## 12: Structure Generation

### Etching

---

## Etching

Three main specifications are required for all etching steps:

- Etching type
- Material or materials to be etched
- Amount of material to be removed

The supported etching types are specified using the `type` argument of the `etch` command.

Table 89 Supported etching types

Etching type	Description
<code>type=angles.rates</code>	Etches according to a definition of a piecewise linear etching rate. See <a href="#">Piecewise Linear Etching on page 783</a> .
<code>type=anisotropic</code>	Etches in the vertical direction only. See <a href="#">Anisotropic and Directional Etching on page 770</a>
<code>type=cmp</code>	Performs chemical-mechanical polishing (CMP). The coordinate of the new surface must be specified as <code>coord</code> . See <a href="#">Polyagonal Etching and CMP on page 774</a>
<code>type=cmp.flat</code>	Similar to CMP, except the new surface specified by <code>coord</code> is flattened following stress relaxation and has zero displacement.
<code>type=crystal</code>	Performs angle-dependent etching where the etching rate depends on the crystallographic direction. See <a href="#">Crystallographic Etching on page 778</a>
<code>type=directional</code>	Etches in one specific direction only. See <a href="#">Anisotropic and Directional Etching on page 770</a> .
<code>type=fourier</code>	Performs angle-dependent etching where the etching rate is a cosine expansion of the etching angle. See <a href="#">Fourier Etching on page 775</a> .
<code>type=isotropic</code>	Performs etching where the etching rate is uniform in all directions. See <a href="#">Isotropic Etching on page 769</a> .
<code>type=polygon</code>	Etches according to a user-supplied polygon (2D operations only). See <a href="#">Polyagonal Etching and CMP on page 774</a> .
<code>type=trapezoidal</code>	Allows etching with undercut and taper angle specifications (2D operations only), or taper and bottom angle specifications (3D operations only). See <a href="#">Trapezoidal Etching on page 779</a>

Some etching types have an option that can be used instead of specifying type:

- `anisotropic` (instead of `type=anisotropic`)
- `cmp` (instead of `type=cmp`)
- `isotropic` (instead of `type=isotropic`)
- `trapezoidal` (instead of `type=trapezoidal`)

Each etching type requires the setting of parameters particular to that type. Many options are available and some options are available only with certain etching types. [Table 90](#) summarizes the syntax options for each etching type.

Table 90 Options for etch command syntax

Area	Parameter name	angles.rates	anisotropic	cmp, cmp.flat	crystal	directional	fourier	isotropic	polygon	trapezoidal
Rate	rate		*			*		*		*
	angles.rates	*								
	coeffs						*			
	mat.coeffs						*			
	crystal.rate				*					
Stop criteria	time	*	*		*	*	*	*		*
	thickness		*			*		*		*
	etchstop	*	*	*	*		*	*		
	coord			*						
	etchstop.overetch	*	*	*	*		*	*		
	isotropic.overetch		*		*					
Shape	polygon								*	
	angle								*	
	undercut									*a
	bottom.angle									*b
	bottom.thickness									*b
	direction				*					
	ambient.rate									*c
Beam	sources	*					*			
	shadowing	*	*c			*	*			
	shadowing.nonisotropic						*			
Mesh	remesh	*	*	*	*	*	*	*	*	
	Adaptive	*	*	*	*	*	*	*	*	
Mode	1D								*	
	force.full.levelset		*		*d	*	*d	*		*

- a. In 2D when not using `force.full.levelset`.
- b. In 3D when not using `force.full.levelset`.
- c. When used in conjunction with `force.full.levelset`.
- d. Full level set is the default scheme for crystallographic and Fourier etching.

## 12: Structure Generation

### Etching

**NOTE** To remove materials exposed to the top gas, use the `strip` command not the `etch` command. The `strip` command is used specifically for this purpose. It is more straightforward, less prone to user error, and more robust in delivering the expected results. For example:

```
strip Photoresist
```

Etching types have been implemented in Sentaurus Process using three different methods (analytic, fast level-set, and general time-stepping level-set), which are described in [MGOALS on page 816](#).

These methods may require different inputs to perform the steps and may take different effects into account. The method is selected depending on the specified parameters and the structure to be etched.

**NOTE** The simplest and fastest algorithm possible is chosen by default.

If simple isotropic, anisotropic, directional, or CMP etching of a single material is requested and for polygonal etching, an analytic method is used. The analytic method is the fastest and most accurate. However, in some cases, the resulting etching front might intersect itself. Sentaurus Process detects such situations and switches to the fast level-set method.

**NOTE** Although analytic methods are fast and can handle most simple etching tasks, they do not consider shadowing or visibility effects, and they cannot etch more than one material at a time.

The general time-stepping level-set method is chosen if you specify any rate versus angle-type etching (Fourier or crystallographic), or if you choose to etch different materials at different rates, or if the option `force.full.levelset` is specified. In addition, the general time-stepping level-set method can handle multiple etching beams and, optionally, shadowing.

The general time-stepping level-set method used in Sentaurus Process has the same limitations as all level-set methods:

- Sharp corners in the evolving front are rounded.
- Small front movement requires a fine level-set mesh, resulting in large memory use and long simulation times.
- The accuracy is limited by the size of the level-set mesh.

Besides the etching type, the materials to be etched and the amount of material to be removed must be specified. The amount of material to be etched can be specified in three ways:

- Thickness
- Rate and time
- Using an etch stop

The etching rate may be specified using etching beams that are created with the `beam` command. Beams can be used only with Fourier etching. If an etch stop is specified, the etching stops as soon as the specified material is exposed to gas.

In addition, a mask specification can be given for all etching types, except CMP and polygonal to limit the areas where material is removed.

**NOTE** Trapezoidal etching supports mask specification in 3D only.

---

## Isotropic Etching

Isotropic etching removes material at the same rate in all directions.

When isotropic etching uses either the fast level-set method or the general time-stepping level-set method, the final surface is obtained by solving a differential equation on a discrete mesh.

**NOTE** To control errors in the fast level-set method, use `resolution` in the `mgoals` command. For the general etch method, use either `resolution` or the `dx` and `dy` arguments of the `mgoals` command.

An example of a single-material isotropic etch is (see [Figure 92](#)):

```
etch silicon thickness= 0.05 type= isotropic
```

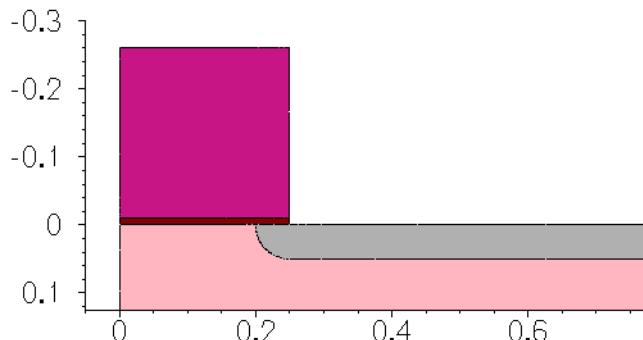


Figure 92 Single-material isotropic etching

## 12: Structure Generation

### Etching

An example of a multimaterial isotropic etch is (see [Figure 93](#)):

```
etch material= {Silicon Oxide Poly} rate= {1.0 1.5 1.0} time= 0.05 \
type= isotropic
```

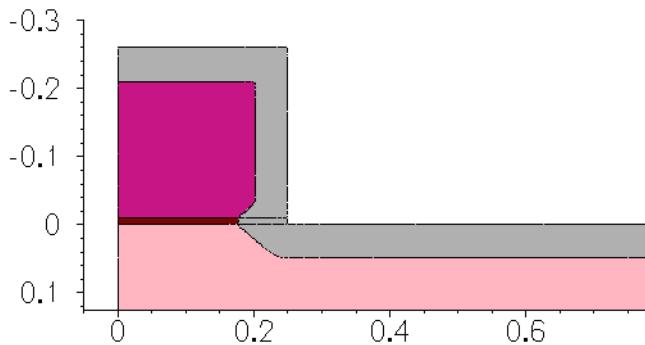


Figure 93 Multimaterial isotropic etching

---

## Anisotropic and Directional Etching

Anisotropic etching is designed to work primarily with masks or masking layers. Anisotropic etching removes material in a direction that is purely vertically downwards (see [Figure 94](#)).

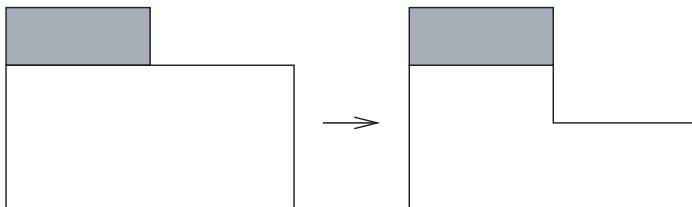


Figure 94 Anisotropic etching

Anisotropic etching can take more than one material if the same rate is specified for all etched materials. This can be useful to create multiple spacers since it does not produce small gaps, which are difficult to avoid when etching one spacer at a time. If you want to use different rates for each material, a better alternative is Fourier etching.

If anisotropic etching is performed to etch the shaded region in the structure shown in [Figure 95](#), instabilities can arise. The resulting structure can be very different depending on the numeric round-off errors.

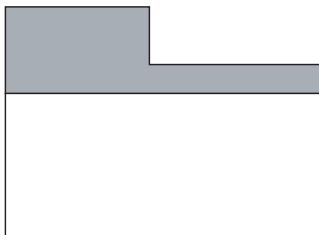


Figure 95 For this structure, anisotropic etching would not be stable

**NOTE** With regard to anisotropic etching:

- Anisotropic operations are sensitive to numeric noise at vertical or nearly vertical walls.
- If the `etch` command is supposed to remove the entire layer, care must be taken to overetch by a small amount to prevent thin regions remaining due to numeric round-off errors.
- It is more robust and better to use the `strip` command to remove all exposed layers of a certain material.

In two dimensions, when anisotropic etching is performed, portions of the etched material lying underneath other material are protected by those materials and, therefore, no etching occurs in those areas. For example, in [Figure 96 on page 772](#), when silicon is etched using anisotropic etching, the portion lying underneath oxide is not etched.

On the other hand, depending on the etching rate, in three dimensions, the silicon area underneath oxide can be etched away, as shown in [Figure 97 on page 772](#). To make the behavior consistent with 2D anisotropic etching, you can specify the `aniso.etching.protect.materials` option of the `mgoals` command:

```
mgoals aniso.etching.protect.materials
```

## 12: Structure Generation

### Etching

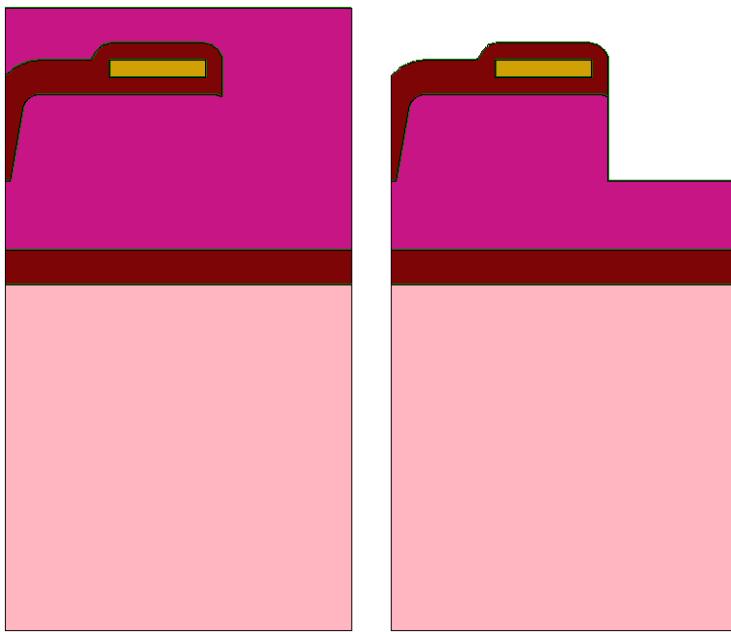


Figure 96 Two-dimensional anisotropic etching with material providing protection:  
(left) original structure and (right) result after etching

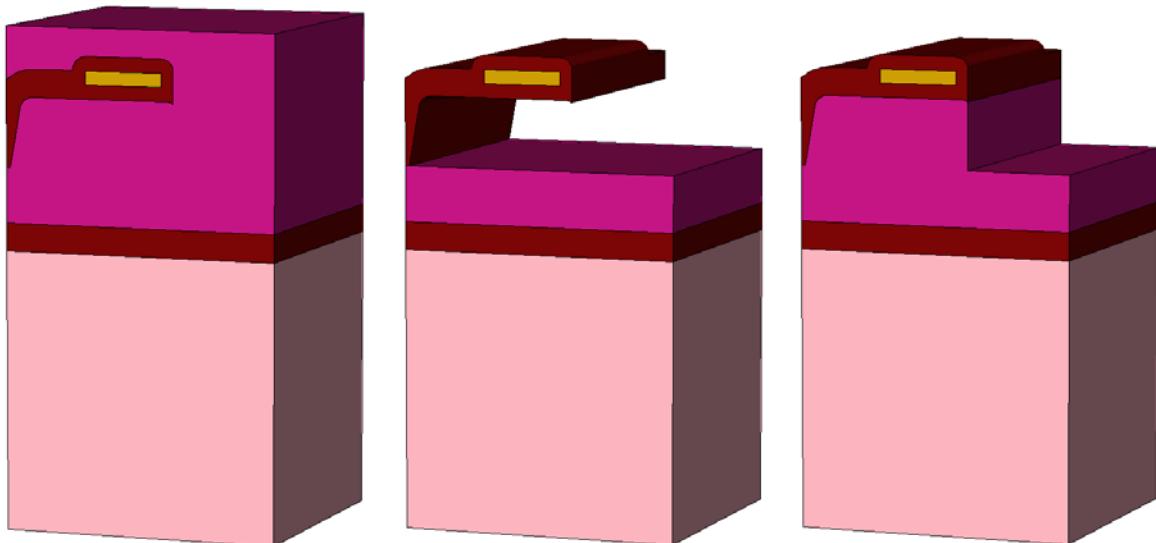


Figure 97 Three-dimensional anisotropic etching with material providing protection:  
(left) original structure, (middle) default behavior leaving a floating region, and  
(right) behavior with `aniso.etching.protect.materials` option

Directional etching is similar to anisotropic etching. In this case, the specified etching rate is applied in the direction of the etching beam. Visibility effects are not considered. The etching window is determined from user-defined masks and from the exposed areas of the etched material (see [Figure 98](#)). For example:

```
etch silicon thickness= 0.05 type= anisotropic
```

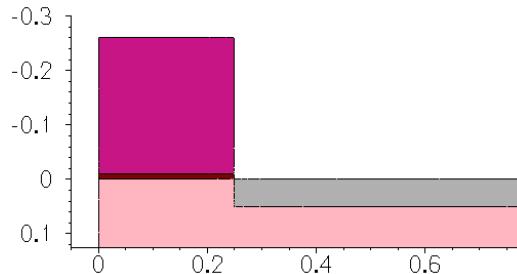


Figure 98 Anisotropic etching

In the next example of directional etching, the argument `direction` specifies the direction of the etching beam by setting values for  $\{x\ y\ z\}$ . This direction vector is normalized to 1.0 before the `etch` command is executed.

```
etch material= silicon rate= 0.05 time= 1.0 type= directional direction= {1 1}
```

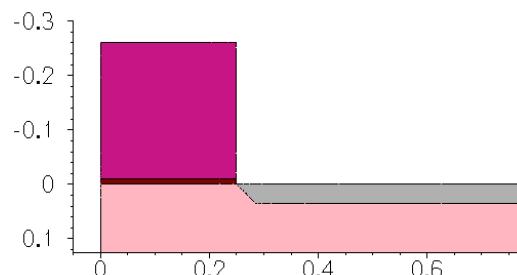


Figure 99 Directional etching (angled wall)

```
etch material= silicon rate= 0.05 time= 1.0 type= directional direction= {1 -1}
```

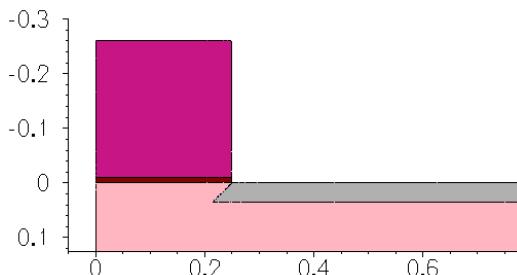


Figure 100 Directional etching with undercut

## 12: Structure Generation

### Etching

## Polygonal Etching and CMP

Polygonal etching provides a way of modifying a region without having to define etching rates or the direction of the etch. The parts of the region inside the polygon that is etched are replaced by gas.

CMP is handled as a special case of polygonal etching. Mesh elements are intersected at the specified coordinate. All elements of the specified material above the coordinate are reassigned to gas.

This example etches a polygon given as  $x_1 \ y_1 \ x_2 \ y_2 \ \dots \ x_n \ y_n$ :

```
etch type= polygon material= silicon \
polygon= {-0.1 0.1 0.05 0.1 0.05 0.6 -0.1 0.6}
```

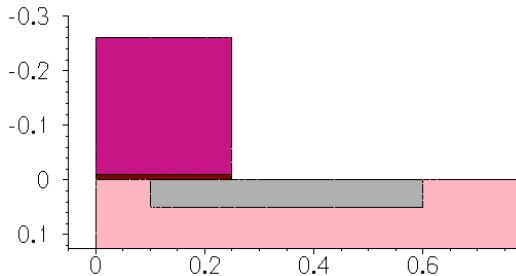


Figure 101 Polygonal etching

For example:

```
etch type= cmp coord= 0.05 material= all
```

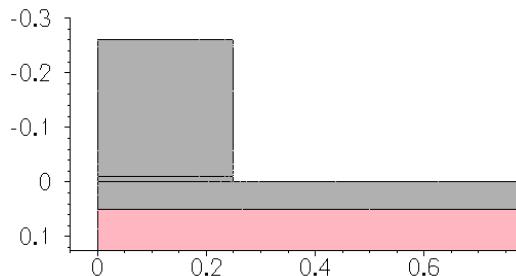


Figure 102 CMP

---

## Fourier Etching

In Fourier etching, the etching rate is a function of the angle between the incident etching beam and the normal vector of the surface being etched. This allows for reasonably directional etching with control of the slope of sidewalls. The coefficients  $A_n$  are defined using `coeffs` (for a single-material etch) or `mat.coeffs` (for a multimaterial etch), and the etching rate is computed according to:

$$\text{etch rate} = \sum_{i=0}^m \text{factor}_i \sum_{j=0}^n A_j \cos^j \theta_i \quad (992)$$

where:

- $\theta_i$  is the angle between the incident beam  $i$  and the normal to the surface being etched.
- $\text{factor}_i$  is the `factor` given in the `beam` command for beam  $i$ .

Any number of coefficients  $A_j$  can be given for each material. If the parameters  $A_j$  are chosen such that negative etching rates would result in some slope angles, no etching will occur on the parts of the surface that have that slope.

It is common to set the parameters  $A_j$  such that the etching rate for angles less than a certain angle are positive and drop below zero (resulting in no etching) above that angle. This produces a trench with a rounded bottom and a sidewall given by the angle where the etching rate drops to zero.

Fourier etching uses the full level-set method formulated after Lax–Friedrichs. This formulation shows good stability, leading to good accuracy of etch wall-angle control. The Lax–Friedrichs formulation results in slightly less corner sharpness.

**NOTE** See the TCAD Sentaurus Tutorial (Sentaurus Process module) for an example of Fourier etching:

[Applications\\_Library/GettingStarted/sprocess/Fourier](#)

The `beam` command defines the direction and the relative strength of etching beams to be used with Fourier etching. The syntax is:

```
beam name=<c> (direction= {<x> <y> <z>} | incidence=<n>) factor=<n>
```

You specify the angle of incidence of each beam using either `direction` (the specified direction vector is normalized automatically to unit length) or `incidence` (`incidence=0` defines a vertical beam).

## 12: Structure Generation

### Etching

The angle  $\theta_i$  in Eq. 992 is measured from the surface perpendicular to the angle of incidence for beam  $i$ . The relative strength factor is the weight (strength) of each beam. Each etching beam must be given a unique name.

Etching beams are assumed to be collimated, that is, a slight angular spread of beam direction is not considered.

The sources argument of the `etch` command lists the names of etching beams to be used in an etching operation.

For example (see Figure 103):

```
beam name= src1 direction= {1 0 0} factor= 1
etch material= silicon type= fourier sources= src1 coeffs= {0 0 1.0} time= 0.05
```

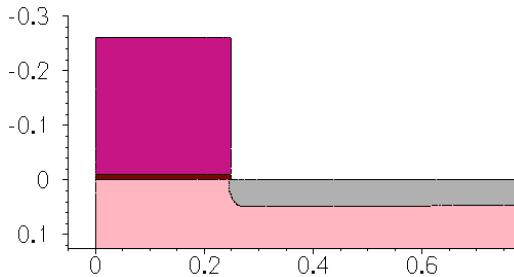


Figure 103 Fourier etching

Through the selection of Fourier coefficients, the angle of the etching wall can be controlled to a large degree. In particular, the first coefficient in the list,  $A_0$ , corresponds to the equivalent of the rate of isotropic etching. The second coefficient in the list,  $A_1$ , corresponds approximately to the equivalent of the rate of anisotropic or directional etching. The approximate formula for determining the etch wall angle is given as:

$$\varphi \approx \cos^{-1} \frac{-A_0}{A_1} \quad (993)$$

where  $\varphi$  is the angle of the etch wall measured from the horizontal plane. For example,  $A_0 = -0.5$  and  $A_1 = 0.7071$  result in an etch wall at an angle of approximately  $45^\circ$  from the horizontal as shown in Figure 104 on page 777:

```
beam name= src1 direction= {0.1 0 0} factor= 1
etch material= {silicon} type= fourier sources= {src1} coeffs= {-0.5 0.7071} \
time= 1.0
```

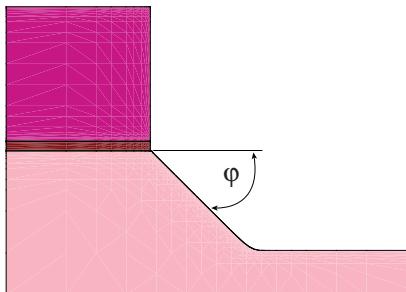


Figure 104 Fourier etching with etch wall angle of 45°

Another Fourier etching example shows the functionality in three dimensions and how multiple rates for multiple materials are specified using `mat.coeffs`. For 3D Fourier etching, also use the command `sde off`.

Etching coefficients chosen for this example are illustrative and might not be physically meaningful:

```
beam name= src1 direction= {1 0 0} factor= 1
etch sources= {src1} type= fourier remesh= false time= 1 \
mat.coeffs= { Silicon= {-1 2} Nitride= {-0.7 1.2} Oxide= {0.01} \
PolySilicon= {-0.05 0.2} }
```

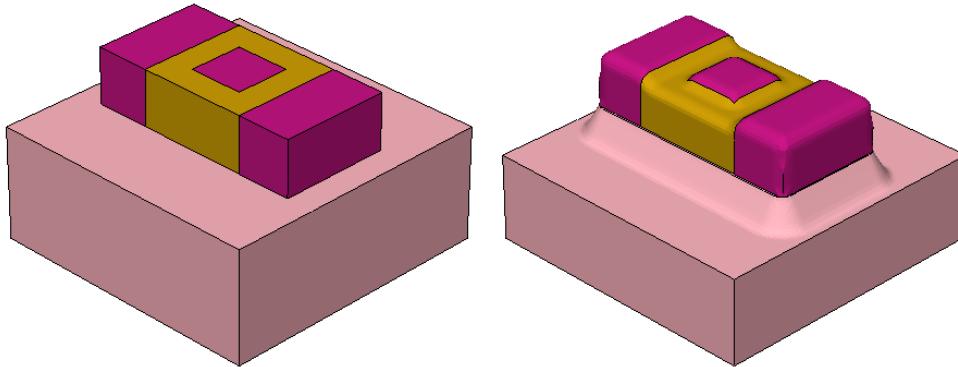


Figure 105 Three-dimensional multimaterial Fourier etching: (*left*) before etching and (*right*) after etching

## The shadowing and shadowing.nonisotropic Options

**NOTE** Shadowing is not implemented in 3D Fourier etching.

The `shadowing.nonisotropic` option is used instead of `shadowing` when you want to allow only the 0th-order Fourier coefficient to etch areas where the beam is shadowed.

## 12: Structure Generation

### Etching

The shadowing option prevents all Fourier etching in areas shadowed from the beam; while the shadowing.nonisotropic option prevents only the Fourier coefficients of order one and higher from etching in areas where the beam is shadowed.

Be aware that even when shadowing is specified, the 0th-order Fourier coefficient  $A_0$  should continue to etch areas where the beam is shadowed. This permits pseudo-isotropic etching that is independent of shadowing, while at the same time, full Fourier etching occurs only in areas where the beam is not shadowed.

---

## Crystallographic Etching

The argument `crystal.rate` defines etching rates for different crystallographic orientations to be used in crystallographic etching (see [Defining the Crystal Orientation on page 41](#)).

Crystallographic etching rates are specified in `crystal.rate` as a list of one or more Miller indices  $i$ ,  $j$ , and  $k$  with corresponding etching rates. The currently supported indices  $\langle ijk \rangle$  are  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ ,  $\langle 111 \rangle$ ,  $\langle 311 \rangle$ ,  $\langle 511 \rangle$ ,  $\langle 911 \rangle$ , and  $\langle 221 \rangle$ :

```
crystal.rate= {"<100>" =<etch_rate> "<110>" =<etch_rate> "<111>" =<etch_rate>}
```

**NOTE** You must add a space between the double quotation mark ("") after the orientation and the equal sign.

Interpolation of the rate at a given point along the etch front is calculated as a linear combination of the  $\langle ijk \rangle$  rates weighted by the component of the etch front normal vector along the corresponding crystallographic direction.

A crystallographic etching example is (see [Figure 106](#)):

```
etch material= silicon type= crystal \
  crystal.rate= {"<100>" =1.0 "<110>" =0.5 "<111>" =0.001} time= 0.25
```

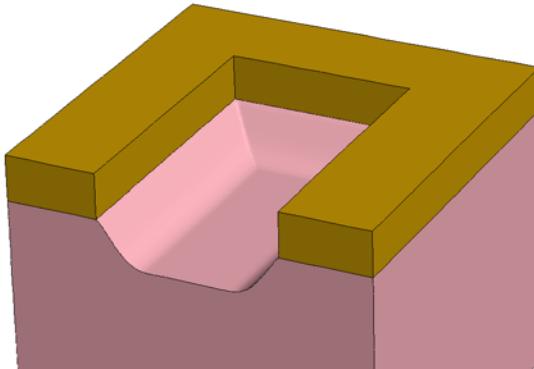


Figure 106 Crystallographic etching

---

## Trapezoidal Etching

Trapezoidal etching provides a simple but flexible approximation to a number of real etching processes. The location of the etch is determined by masking layers (that is, layers of nonetchable material that, if nonexistent, can be easily created with the photo command). In three dimensions, the etch location can be specified through the definition of a mask.

Trapezoidal etching uses the following arguments to specify the shape of the region to be removed:

- `thickness` specifies the vertical depth (or a combination of `rate` and `time`).
- `angle` specifies the angle (in degrees) of the resulting sidewalls.
- `undercut` specifies the horizontal penetration of the etch under the edges of the masking layer. It only works in two dimensions.
- `bottom.angle` and `bottom.thickness` specify the angle and thickness of the sidewalls for a second etching after thickness and angle are already etched (3D operations only).

These arguments can be used to approximate a number of real etching processes including:

- Combinations of vertical and isotropic etches.
- V-groove etches.
- Etches that produce retrograde sidewall profiles.

### Two-Dimensional Trapezoidal Etching

Trapezoidal etching is performed as follows:

1. Perform vertical etching to depth `thickness`. This etching does not apply to portions of the surface that are masked by nonetchable materials or shadowed by etchable or nonetchable materials. In addition, it is not used on segments of the surface that form an angle greater than `angle` to the horizontal.
2. Perform horizontal etching. Surfaces that were exposed at the start of Step 1 are etched horizontally by the distance `undercut`. Surfaces that were exposed during Step 1 are etched by a distance proportional to the length of time between when they first became exposed and the end of Step 1. Therefore, a sidewall exposed three-fourths of the way into Step 1 is etched horizontally by one-fourth of `undercut`. (An exception is made when an angle greater than 90° is specified.)
3. Perform a vertical upwards etch (that is, in the direction) where overhangs of etchable material are present at the end of Step 2. On surfaces that were exposed at the start of Step 2, this etching is to a distance `undercut`. On surfaces that were first exposed during Step 2, the distance of this etching is reduced in proportion to the time from the start of

## 12: Structure Generation

### Etching

Step 2. This step approximates the undercutting of the mask due to the isotropic component of the etching.

**NOTE** Trapezoidal etching using a mask definition is not supported in 2D operations.

When the thickness, angle, and undercut arguments satisfy the following relationship, the etching approximates a vertical etching with an isotropic component:

$$\text{thickness} = \text{undercut} \cdot \tan(\text{angle}) \quad (994)$$

This is the case whenever two or fewer of these arguments are specified with the `Trapezoidal.Etch.Undercut` parameter switched on (default is 0):

```
pdbSet Grid Trapezoidal.Etch.Undercut 1
```

For example:

```
etch material= silicon type= trapezoidal thickness= 0.25 undercut= 0.1
```

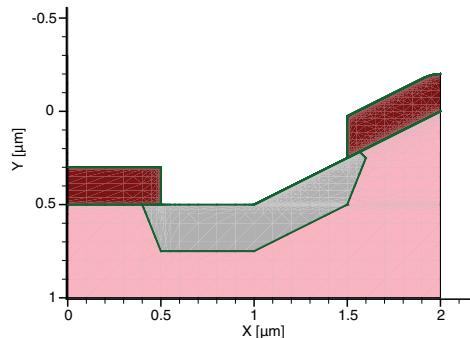


Figure 107 Basic trapezoidal etching example where the surface is nonplanar

The left half of [Figure 107](#) shows the result when etching a planar substrate. The etch region is a trapezoid of depth `thickness`, extending a distance `undercut` beneath the mask edge. The right half of [Figure 107](#) shows the result when etching a nonplanar surface.

Step 1 of the sequence etches the exposed surface vertically to a depth of `thickness` micrometers. Step 2 etches the resulting sidewall in the horizontal direction, producing an undercutting of the mask and the sloped sidewall. In this case, Step 3 also has an effect, etching upwards from the undercut region. Therefore, the hook in the final silicon profile is the result of approximating the isotropic component of the etch. In each case, the intersection between the bottom of the etched region and the sidewall occurs directly under the edge of the mask.

[Figure 108](#) and [Figure 109](#) on page 781 show what happens when Eq. 994 is not satisfied.



Figure 108 Trapezoidal etching example generating a narrow trench bottom

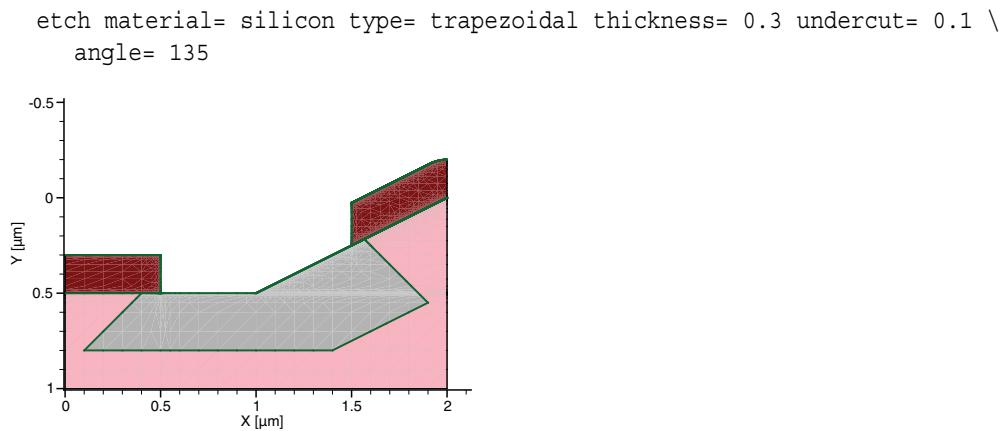


Figure 109 Trapezoidal etching example generating a wide trench bottom

In [Figure 108](#), thickness/undercut are less than  $\tan(\text{angle})$ . In this case, the sloped sidewall of the etch extends out under the opening in the mask. The intersection between the bottom of the etch region and the sidewall is no longer directly beneath the edge of the mask. If the mask opening is narrow enough, the bottom of the etch region disappears entirely, resulting in a V-groove etch. To produce this etch shape, Step 1 of the etch process is modified to reduce the depth of the vertical etch near the edges of the mask opening. Note that, in this situation, even the smallest amount of nonetchable material can produce a triangular mound of unetched material in the final structure.

[Figure 109](#) shows the case with an angle greater than  $90^\circ$ . In this case, the bottom of the etched region is wider than the opening in the masking layer, producing overhanging sidewalls. This etch is accomplished by modifying Step 2 of the procedure to etch further horizontally at the bottom of the sidewalls formed by Step 1 than at the top. The apparent etch depth of  $0.5\ \mu\text{m}$  at the right side of the mask opening is the result of a  $0.3\ \mu\text{m}$  vertical etch of the original sloped surface (Step 1) followed by a  $0.4\ \mu\text{m}$  horizontal etch of the sloped ‘bottom wall’ that results from Step 1.

## 12: Structure Generation

### Etching

## Three-Dimensional Trapezoidal Etching

There are two possible cases for 3D trapezoidal etching:

- Case 1: A thickness (or rate and time) and an angle (optional) are specified. If angle is not specified, it defaults to  $90^\circ$  (vertical). In contrast with case 2, angle allows any value between  $0^\circ$  and  $180^\circ$ . [Figure 110](#) shows examples of both cases.
- Case 2: A thickness (or rate and time), an angle (optional), and bottom.thickness and bottom.angle (optional) are specified. If angle is not specified, it defaults to  $90^\circ$  (vertical). Here, a special condition applies: angle must be greater than or equal to  $90^\circ$ , while bottom.angle must be smaller than or equal to  $90^\circ$ . That is, the *first etching* penetrates behind the mask, while the second one does the opposite. [Figure 111](#) shows an example of this type.

**NOTE** For 3D trapezoidal etching to succeed, the initial etching surface must be flat.

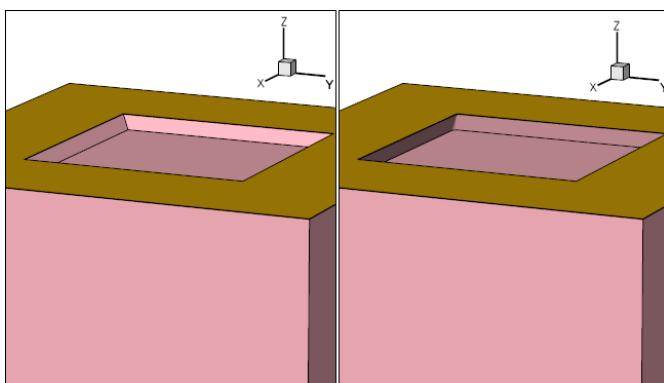


Figure 110 Three-dimensional trapezoidal etching: (*left*) angle=45 thickness=0.3 and (*right*) angle=110 thickness=0.44

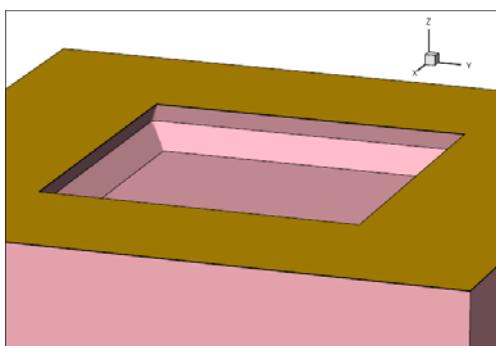


Figure 111 Three-dimensional trapezoidal etching produced with angle=110, thickness=0.3, bottom.angle=45, and bottom.thickness=0.400

## Trapezoidal Etching Using force.full.levelset Option

When the `force.full.levelset` option is specified for trapezoidal etching:

- The etching depth is controlled by `rate` and `time`, not by `thickness`.
- The argument `ambient.rate` is used to approximate the underetch effect otherwise available in the non-`force.full.levelset` case controlled in two dimensions by `undercut`. If `undercut` is specified, `ambient.rate` will be approximated by `undercut/time`, and a warning message will be issued. The `ambient.rate` argument also approximates underetching, controlled in three dimensions in the non-`force.full.levelset` case by the combination of `angle`, `bottom.angle`, and `bottom.thickness`.
- The options supported by the level-set solver such as `shadowing` become available.
- An additional argument `roundness` (default 1.0) can be used to increase the curvature of etching sidewalls.

## Piecewise Linear Etching

In piecewise linear etching, the etching rate is a user-defined piecewise linear function of the angle between the incident etching beam and the normal vector of the surface being etched. You define the points of angle versus rate on a material-by-material basis, as per the following syntax:

```
angles.rates= {
    matA = {angleA0 rateA0 angleA1 rateA1 ... angleAn rateAn}
    matB = {angleB0 rateB0 angleB1 rateB1 ... angleBn rateBn}
    ...
}
```

where  $\text{angle}_{n-1} \leq \text{angle}_n$ .

The rates and angles are interpreted as follows:

- Angles are given in degrees in the range  $[0^\circ, 180^\circ]$ .
- The rate for  $\text{angle} < \text{angle}_0$  is  $\text{rate}_0$ .
- The rate for  $\text{angle} > \text{angle}_n$  is 0.
- The rate is calculated as the linear interpolation of the nearest two angle–rate pairs within which the angle lies.

While Fourier etching and trapezoidal etching also define the etching rate according to the angle between the beam direction and the surface normal, a piecewise linear function is a more general parameterization of etching rate versus angle that users control directly.

## 12: Structure Generation

### Etching

For example (see [Figure 112](#)):

```
beam name= src1 direction= {1 0 0} factor= 1
etch type= angles.rates sources= src1 time= 0.2 \
    angles.rates= { Silicon= { 25 1.0 45 0.3 } }
```

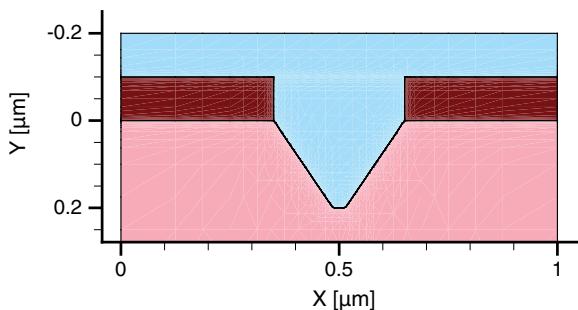


Figure 112 Piecewise linear etching

You must define the piecewise linear function as smoothly as possible, avoiding discontinuous changes, to ensure well-defined level-set results.

### Etching Beams

The `beam` command defines the direction and the relative strength of etching beams to be used with piecewise linear etching (see [Fourier Etching on page 775](#)).

The argument `sources` of the `etch` command lists the names of etching beams to be used in an etching operation.

---

## Etching Tips

Some tips for etching are:

- If the total etch thickness is exactly the same thickness as the layer to be etched, numeric round-off errors can cause thin pieces of the material to be retained. You should etch a little more (for example, 0.1%) than the thickness of the layer.
- Etching small thicknesses using a small `isotropic.overetch` or etching large structures can cause the simulation to allocate a large amount of memory and to increase the simulation time to solve the level-set equation. The argument `resolution` of the `mgoals` command can be increased for the simplified boundary movement mode, and the arguments `dx` and `dy` can be increased in the general boundary movement mode to reduce memory consumption. However, this may affect accuracy.

---

## Deposition

Three main specifications are required for all deposition steps:

- Deposition type
- Material to be deposited
- Amount of material to be deposited

The supported deposition types are specified using the `type` argument of the `deposit` command.

**Table 91** Supported deposition types

Deposition type	Description
<code>type=anisotropic</code>	Performs anisotropic deposition.
<code>type=crystal</code>	Performs crystallographic deposition. The <code>crystal.rate</code> argument must be specified. See <a href="#">Crystallographic Deposition on page 789</a> .
<code>type=directional</code>	Performs anisotropic deposition using a specified direction.
<code>type=fill</code>	Performs a fill of the structure with the specified material up to the coordinate specified with the argument <code>coord</code> . See <a href="#">Polygonal Deposition and Fill on page 788</a> .
<code>type=fourier</code>	Performs Fourier deposition. See <a href="#">Fourier Deposition on page 790</a> .
<code>type=isotropic</code>	Performs isotropic deposition. See <a href="#">Isotropic Deposition on page 788</a> .
<code>type=polygon</code>	Performs a polygonal deposition that requires the <code>polygon</code> argument. The specified polygon is used to intersect all mesh elements of material gas. Then, elements inside the polygon are assigned to the specified material. (Not available in 3D operations.) See <a href="#">Polygonal Deposition and Fill on page 788</a> .
<code>type=trapezoidal</code>	Performs a trapezoidal deposition that requires the <code>angle</code> and <code>thickness</code> arguments (3D operations only). See <a href="#">Trapezoidal Deposition on page 790</a>

Some deposition types have an option that can be used instead of specifying `type`:

- `anisotropic` (instead of `type=anisotropic`)
- `crystal` (instead of `type=crystal`)
- `fill` (instead of `type=fill`)
- `fourier` (instead of `type=fourier`)
- `isotropic` (instead of `type=isotropic`)

## 12: Structure Generation

### Deposition

Each deposition type requires the setting of parameters particular to that type. Many options are available and some options are available only with certain deposition types. [Table 92](#) summarizes the syntax options for each deposition type.

Table 92 Options for deposit command syntax

Area	Parameter name	anisotropic	crystal	directional	fill	fourier	isotropic	polygon	trapezoidal
<b>Rate</b>	rate	*		*			*		
	coeffs					*			
	mat.coeffs					*			
	crystal.rate		*						
<b>Stop criteria</b>	time	*	*	*		*	*		
	thickness	*		*			*		*
	coord				*				
<b>Shape</b>	polygon							*	
	angle								*
	direction			*					
<b>Beam</b>	sources					*			
	shadowing	*		*		*			
	shadowing.nonisotropic					*			
<b>Mesh</b>	remesh	*	*	*		*	*	*	
	Adaptive	*	*	*		*	*	*	
<b>Mode</b>	1D							*	
	force.full.levelset		* <sup>a</sup>	*		* <sup>a</sup>	*		

a. Full level set is the default scheme for crystallographic and Fourier deposition.

To specify the thickness of the deposited layer for anisotropic and isotropic deposition, use either `thickness` or `rate` and `time`. Besides the deposition type and thickness, you must specify the material to be deposited (only one material is allowed per `deposit` command). To do this, either specify the material name (`<material>`) or `material=<c>` in the command.

The number of steps for a deposition is specified using `steps=<n>`. The specified `time` or `thickness` is subdivided accordingly. Subdividing a deposition into several steps might be useful if stresses are initialized in the deposited layer. A stressed film of a given thickness can be deposited at the same time or in several steps. Sentaurus Process simulates stress rebalancing after each deposition step.

Multistep deposition is known to generate more realistic stress profiles compared to depositing the entire layer and then performing one stress rebalancing calculation.

By default, the material is deposited on the surface exposed to the upper gas region. If a structure has buried gas bubbles, they remain untouched. To deposit inside these gas bubbles:

- Specify the `fill.buried` option in the `deposit` command to fill all gas bubbles with the deposited material.
- Specify the `fill.buried.match.surrounding` option in the `deposit` command to fill all gas bubbles with the material surrounding them, while leaving bubbles at a material interface filled with gas. This option will override the behavior of `fill.buried` if it also is specified.
- Specify `fill.buried.interface=<material>` in the `deposit` command to fill all gas bubbles at a material interface with the specified material, *but only* if the material is already present in the simulation (for example, silicon).

The name of a mask also can be specified in the `deposit` command. In this case, the material is deposited outside the specified mask. Deposition inside a mask requires the mask to be inverted by specifying `negative` in the `mask` command defining the mask (see [Photoresist Masks on page 805](#)).

For deposition, the analytic method, the fast level-set method, and the full level-set method are available.

In two dimensions, the analytic method is preferred for performing deposition, and the level-set method is used when the analytic method is not possible because a front collision is detected.

In three dimensions, the analytic method is used for anisotropic deposition, the fast level-set method is used for isotropic deposition, and the full level-set method is used for Fourier deposition.

In the newly deposited region, constant field values can be initialized. For isotropic deposition, you can define piecewise linear solution fields as a function of the distance from the original surface.

## 12: Structure Generation

### Deposition

---

## Isotropic Deposition

For simple, conforming, isotropic deposition, the boundary is offset an equal distance in all directions. For example (see [Figure 113](#)):

```
deposit nitride thickness= 0.05 type= isotropic
```

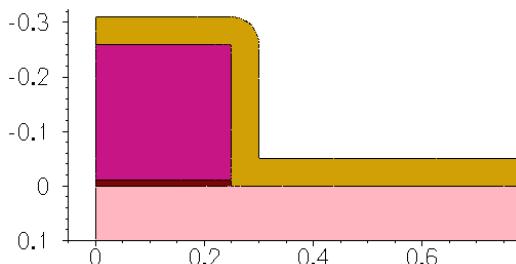


Figure 113 Isotropic deposition

---

## Polygonal Deposition and Fill

Polygonal deposition allows you to deposit polygonal shapes. The corners must be specified as pairs of xy coordinates. Existing non-gas regions will not be overwritten.

**NOTE** Polygonal deposition is not available in 3D simulations.

For example (see [Figure 114](#)):

```
deposit type= polygon material= nitride polygon= {0.1 0.1 0.1 0.6 -0.31 \
0.6 -0.31 0.1}
```

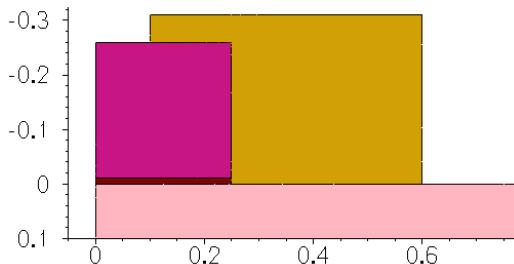


Figure 114 Polygonal deposition

Fill is a special case of polygonal deposition. Only the topmost coordinate must be specified. The simulation domain will be filled up to that coordinate with the specified material.

For example (see [Figure 115](#)):

```
deposit material= nitride type= fill coord= -0.31
```

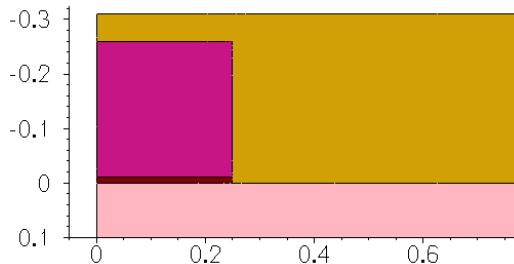


Figure 115 Fill deposition

---

## Crystallographic Deposition

Crystallographic deposition uses the full level-set method to grow single materials whose rate of growth is determined by the crystallographic directions. The crystal is assumed to be cubic regardless of the material being deposited. Deposition rates can be set for one or more of the directions  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ ,  $\langle 111 \rangle$ ,  $\langle 311 \rangle$ ,  $\langle 511 \rangle$ ,  $\langle 911 \rangle$ , and  $\langle 221 \rangle$ . These rates will be applied to their respective equivalent directions based on cubic symmetry, for example, the  $\langle 100 \rangle$  rate will apply to the  $\langle 010 \rangle$ ,  $\langle 001 \rangle$ ,  $\langle \bar{1}00 \rangle$ ,  $\langle 0\bar{1}0 \rangle$ , and  $\langle 00\bar{1} \rangle$  directions.

For example (see [Figure 116](#)):

```
deposit type= crystal material= nitride time= 0.05 \
crystal.rate = {"<100>" =1.0 "<110>" =0.1 "<111>" =0.05}
```

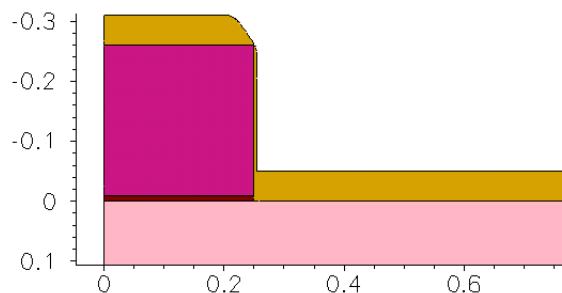


Figure 116 Crystallographic deposition: vertical direction is  $\langle 100 \rangle$ , lateral direction is  $\langle 011 \rangle$

Crystallographic deposition also can be simulated using an atomistic technique (see [Chapter 6](#) on page 567).

---

## Fourier Deposition

Fourier deposition uses the full level-set method to grow single materials whose rate of growth is defined by a function of the angle between the surface normal of the material boundary and the deposition beams. The definition and calculation of the deposit shape are exactly analogous to Fourier etching (see [Fourier Etching on page 775](#)).

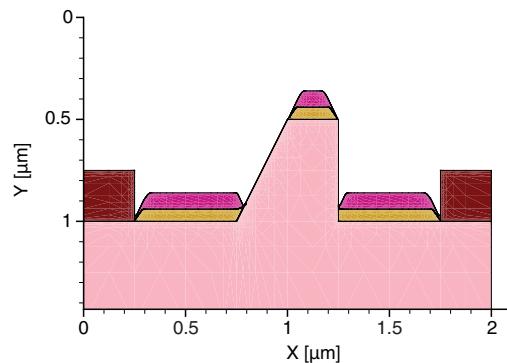
For Fourier deposition, first, define the deposition beam in the same way as in Fourier etching:

```
beam name=<c> (direction= {<x> <y> <z>} | incidence=<n>) factor=<n>
```

Use the `sources` and `coeffs` arguments in the same way as in Fourier etching, for example:

```
beam name= src1 direction= {1 0 0} factor= 1
deposit nitride time= 0.2 fourier sources= {src1} coeffs= { -0.3 0.7 }
```

The `coeffs` argument is given in units of  $\mu\text{m}/\text{minute}$ . By default, `time` is given in minutes.



**Figure 117** Two-dimensional Fourier deposition for demonstration purposes, nitride is deposited selectively on silicon using Fourier deposition and, then, an additional Fourier deposition step adding polysilicon selectively on nitride is performed

---

## Trapezoidal Deposition

Trapezoidal deposition creates a shape with sidewalls of a defined height and angle. Height is defined by `thickness`. Angle is defined by `angle`, measured in degrees from the horizontal, where:

- `angle = 90°` is vertical.
- `angle > 90°` spreads outward as height increases.
- `angle < 90°` closes inward with increasing height.

**NOTE** Trapezoidal deposition is available only in three dimensions.

Separate outward and inward deposition steps can be used to create diamond-like shapes. Trapezoidal deposition requires a flat starting surface, for which `type=fill` can be used.

The following example demonstrates the syntax, whose results are shown in [Figure 118](#):

```
# First step deposition
deposit material= PolySilicon type= trapezoidal \
    selective.materials= Silicon thickness= 0.25 angle= 120

# Provide flat surface for second step
deposit type= fill coord= -0.25 Resist

# Second step deposition
deposit material= PolySilicon type= trapezoidal \
    selective.materials= PolySilicon thickness= 0.25 angle= 60
```

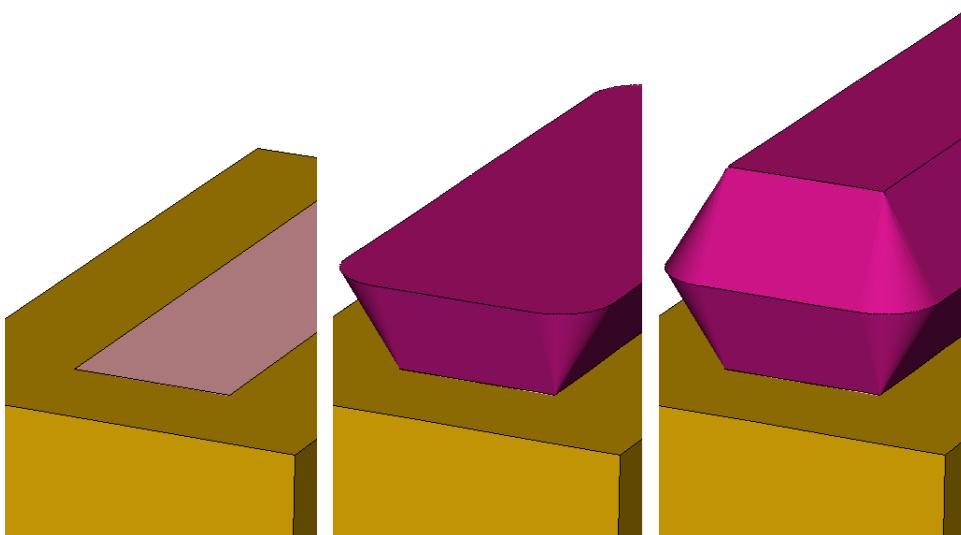


Figure 118 Trapezoidal deposition: (*left*) before deposition, (*middle*) first deposition step with `angle=120`, and (*right*) second deposition step with `angle=60`

---

## Selective Deposition

Selective deposition is optionally available and can be used with isotropic, anisotropic, or Fourier deposition.

Using the `selective.materials` argument, you can select one or more materials to seed growth of the overlayer. In 3D SDE mode, only one material can be specified using `selective.materials`.

## Fields in Deposited Layers

For isotropic deposition, piecewise linear fields can be specified in the deposited layer. For crystallographic deposition, piecewise linear fields with time also can be specified. A doping command must be used for each field; each doping command must assign a unique name.

For example, the following commands create a linear Ge field in the newly deposited oxide layer. Depth 0 corresponds to the initial surface (the bottom of the new layer):

```
doping name= strainGe field= Germanium depths= {0 0.1} values= {1e22 1e22}
deposit material= silicon doping= {strainGe} type= isotropic thickness= 0.1
```

The following commands create a linear boron field in the newly deposited silicon layer:

```
doping name=gradB field=Boron times= {0.0 0.015} values= {1e20 3e20}
deposit type=crystal doping= {gradB} material=Silicon time= 0.015 \
crystal.rate= {<100>=1.0 <110>=0.5 <111>=0.9} selective.materials=Silicon
```

Constant field values can be defined for all deposition types as follows:

```
deposit material= silicon type= isotropic thickness= 0.1 \
fields.values= {Vacancy=1e10 Germanium=2e22}
```

**NOTE** To create layers with intrinsic stress, use the field names StressSELXX, StressELXY, StressELYY, StressSELZZ, StressELYZ, and StressELXZ. It is not necessary to specify all components of stress. Those that are not specified are assumed to be initially at zero. If stresses are added in this way, they will be rebalanced after the deposition is completed. The actual value of the stress may differ from the value that was deposited.

Constant concentrations can be defined for known solution fields (known solution fields must have been defined before the deposit command, either in the SPROCESS.models file or the command file of the user) as:

```
deposit material= {silicon} type= isotropic thickness= 0.1 Vacancy \
concentration= 1e10
```

---

## Handling Stress in Etching and Deposition

In addition to optionally including an automatic ramp-up or ramp-down before etching and deposition, by default, Sentaurus Process automatically rebalances the stresses after etching and deposition. This updates the stress fields at the temperature of the etching or deposition step based on the new geometry.

For the best stress results, you must control the temperature history. This includes thermal ramp-up to process temperature, back to room temperature, and similarly ramp-up and ramp-down for both etching and deposition. However, as a minimum, the elastic stress rebalancing can be handled automatically by switching on stress history (see [Automated Tracing of Stress History on page 711](#)).

It is sometimes useful to switch off this stress rebalancing step in 3D simulations because the rebalance triggers a new mesh to be created. Therefore, if you are more concerned about simulation time than stress accuracy, you should specify the following to allow multiple etching and deposition steps to be performed without a mesh being generated in between:

```
pdbSet Mechanics EtchDepoRelax 0
```

---

## Suppressing Mesh Generation in 3D Simulations

During typical operations in three dimensions, a new mesh is generated only when necessary to perform a task that requires a mesh. Operations such as etching and deposition are performed on the boundary representation and do not necessarily require a new mesh to be generated. However, mechanics steps such as stress rebalance and initializing fields in newly deposited layers do require a new mesh be generated.

By default, a mechanics step is performed after etching and deposition steps to balance the stresses after the structure has changed. The parameter `Mechanics EtchDepoRelax` controls this behavior. In addition, the parameter `Mechanics StressHistory` controls whether a stress rebalance step is added before `etch`, `deposit`, and `diffuse` commands. Either of these rebalance steps can trigger the generation of a new mesh.

If there are multiple etching and deposition steps in sequence, depending on the mechanics material models being used and the thermal history, it may be a good approximation to delay stress rebalancing until after the last step. This can be accomplished with the `suppress.remesh` option of the `etch` and `deposit` commands. Except for the case of deposition with field initialization, which requires a new mesh, this option will suppress mesh generation before and after etching and deposition steps.

**NOTE** When using `suppress.remesh`, be aware that stresses will not be rebalanced if the mesh is out-of-date because of a boundary change.

## Shape Library

The shape library provides commands for generating special-shaped polyhedra in Sentaurus Process. Sentaurus Structure Editor creates these shapes. The shape library is an interface to use those shapes in Sentaurus Process.

There are two ways to use shapes from the shape library:

- In MGOALS mode, polyhedra are created using Sentaurus Structure Editor. The generated polyhedra then can be inserted into a Sentaurus Process structure using the `insert` command.
- In SDE mode, polyhedra are not created directly. Instead, the Sentaurus Structure Editor structure itself is modified by inserting the shapes (replacing other materials). To activate the SDE mode, use the command `sde on`.

The commands available in the shape library are:

- `PolyHedronSTI` creates a shallow trench isolation (STI)-shaped polyhedron.
- `PolyHedronSTIaccc` creates an STI concave active corner-shaped polyhedron.
- `PolyHedronSTIaccv` creates an STI convex active corner-shaped polyhedron.
- `PolyHedronCylinder` creates a cylinder-shaped polyhedron.
- `PolyHedronEllipticCylinder` creates an elliptic cylinder-shaped polyhedron.
- `PolygonSTI` creates a 2D STI-shaped polygon.
- `PolygonWaferMask` creates a wafer mask polygon.
- `PolyHedronEpiDiamond` creates an epitaxial diamond-shaped polyhedron.

You can define additional commands that create parameterized custom shapes using the scripting capabilities of Sentaurus Process and Sentaurus Structure Editor.

---

## PolyHedronSTI

The `PolyHedronSTI` command creates an STI-shaped polyhedron.

The syntax is:

```
PolyHedronSTI name direction X0 Y0 Depth Zmin Zmax Tsti Asti Hsti Rd Rb Ru  
[material]
```

where:

- name is the name of the polyhedron.
- direction can be left, right, front, or back, which sets the facing direction of the STI polyhedron.
- material is optional and specifies the material of the inserted shape in SDE mode. In MGOALS mode, the material of the inserted shape can be specified in the insert command.
- [Figure 119](#) describes the other parameters.

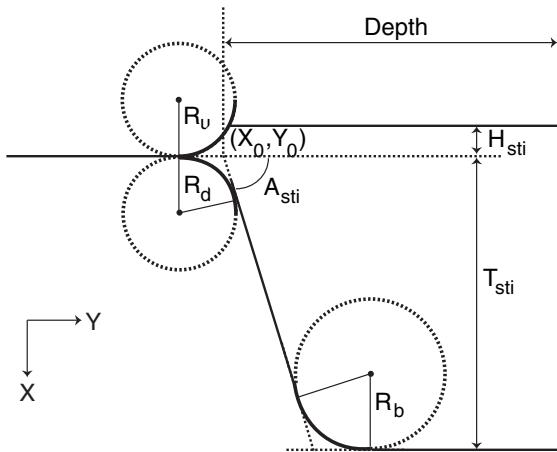


Figure 119 Parameters for generating STI-shaped polyhedron

## 12: Structure Generation

### Shape Library

[Figure 120](#) shows some generated STI shapes in different directions.

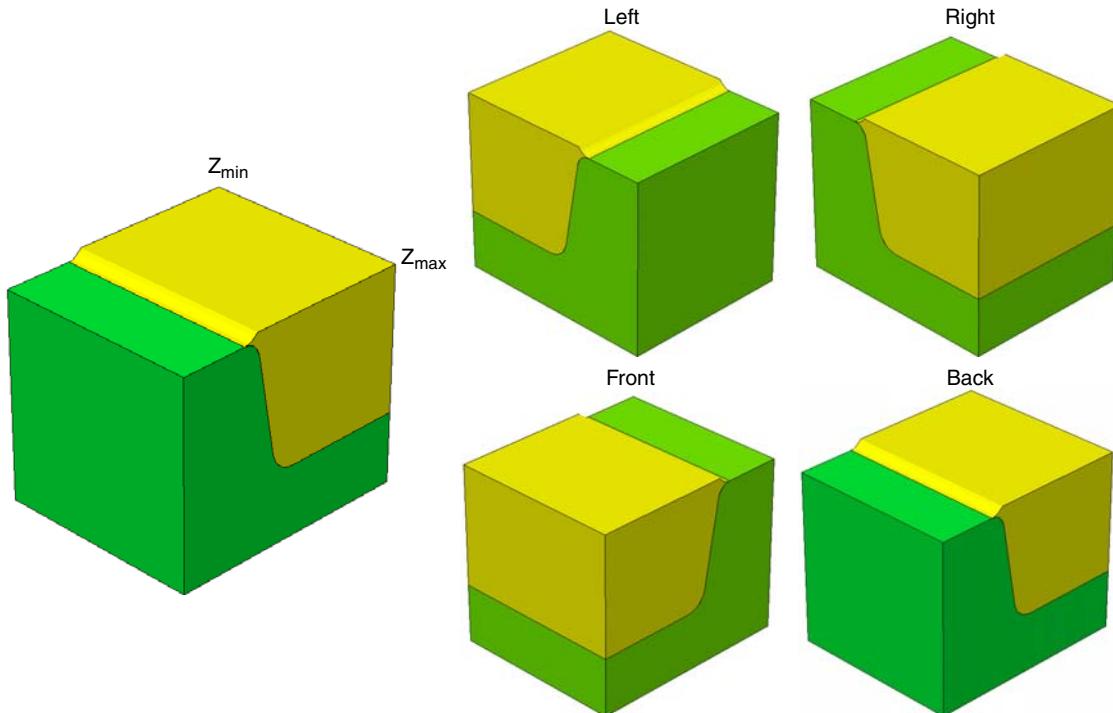


Figure 120 STI-shaped polyhedra in different directions

[Figure 121](#) shows STI shapes with different T<sub>sti</sub> and R<sub>b</sub> values.

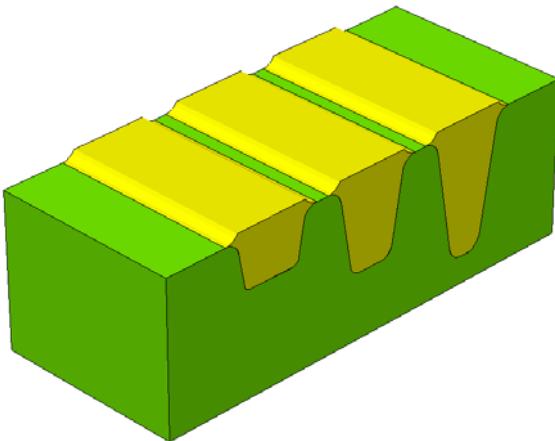


Figure 121 STI-shaped polyhedra with different T<sub>sti</sub> and R<sub>b</sub>

## PolyHedronSTIaccc

The PolyHedronSTIaccc creates an STI concave active corner-shaped polyhedron.

The syntax is:

```
PolyHedronSTIaccc name direction X0 Y0 Z0 Tsti Asti Hsti Rd Rb Ru Rac  
[material]
```

where:

- name is the name of the polyhedron.
- direction can be rb (right back), lb (left back), lf (left front), or rf (right front).
- Rac is the radius of the STI concave corner.
- [Figure 119 on page 795](#) describes the other parameters.

[Figure 122](#) shows STI concave corner-shaped polyhedra in different directions.

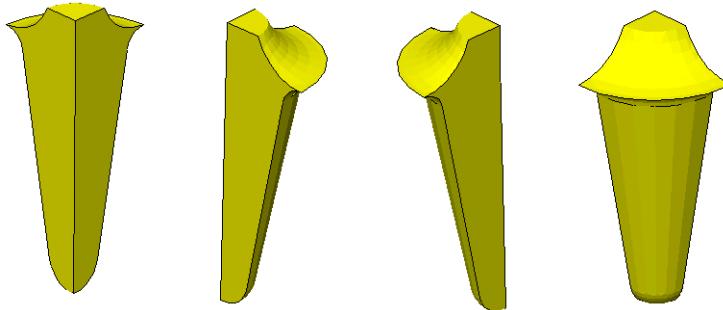


Figure 122 STI concave corner-shaped polyhedra in different directions: (from left to right)  
left back, right back, left front, and right front

## PolyHedronSTIaccv

The PolyHedronSTIaccv command creates an STI convex active corner-shaped polyhedron.

The syntax is:

```
PolyHedronSTIaccv name direction X0 Y0 Z0 Depth Tsti Asti Hsti Rd Rb Ru Rac  
[material]
```

where:

- name is the name of the polyhedron.
- direction can be rb, lb, lf, or rf (as for the PolyHedronSTIaccc command).

## 12: Structure Generation

### Shape Library

- $R_{AC}$  is the radius of the convex corner.
- [Figure 119 on page 795](#) describes the other parameters.

[Figure 123](#) shows a generated STI convex corner-shaped polyhedron.

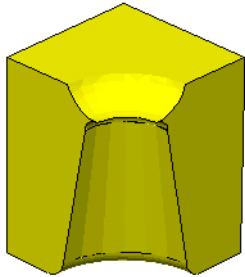


Figure 123 STI convex corner-shaped polyhedron

[Figure 124 \(left\)](#) shows a structure generated by combining the above three STI commands.  
[Figure 124 \(right\)](#) illustrates the directions of the STI shapes.

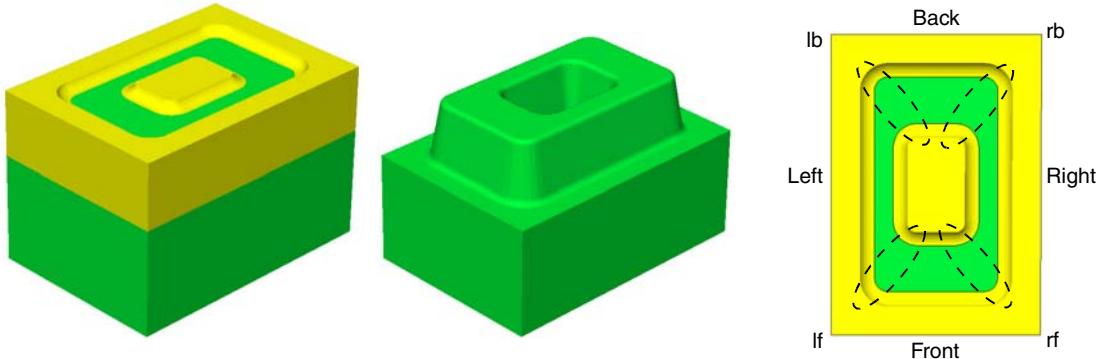


Figure 124 (Left) STI structures and (right) polyhedron directions

---

## PolyHedronCylinder

The PolyHedronCylinder command creates a cylinder-shaped polyhedron.

The syntax is:

```
PolyHedronCylinder name X0 Y0 Z0 Rc Hc [material] [Rotate.Y | Rotate.Z] [angle]
```

where:

- name is the name of the polyhedron.

- If Rotate.Y is specified, the cylinder is rotated at position ( $x_0, y_0, z_0$ ) along the y-axis for angle degrees. If Rotate.Z is specified, the cylinder is rotated along the z-axis. The right-hand rule determines the direction of the rotation.
- angle is the rotation angle in degree.
- Other parameters give the center coordination, the radius, and the height for the cylinder (see [Figure 125](#)).

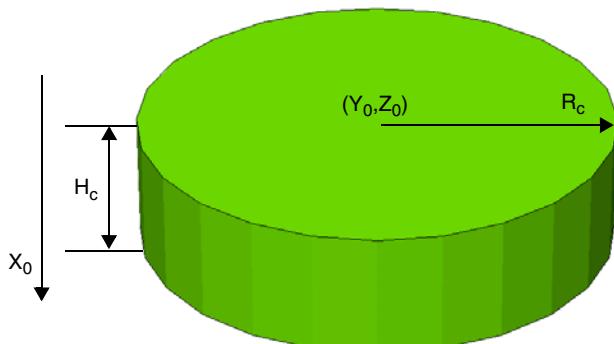


Figure 125 Cylinder-shaped polyhedron

## PolyHedronEllipticCylinder

The PolyHedronEllipticCylinder command creates an elliptic cylinder-shaped polyhedron.

The syntax is:

```
PolyHedronEllipticCylinder name X0 Y0 Z0 Y1 Z1 Ratio Hc [material]
[Rotate.X | Rotate.Y | Rotate.Z] [angle]
```

where:

- name is the name of the polyhedron.
- $x_0, y_0, z_0$  are the center coordinates of the base ellipse.
- $y_1$  and  $z_1$  are the y- and z-coordinates of the major axis of the base ellipse. The base ellipse is on the yz plane.
- Ratio is the ratio of the minor axis to the major axis.
- Hc is the height for the cylinder. The cylinder is extruded in the -x-direction.
- If Rotate.X is specified, the cylinder is rotated at position ( $x_0, y_0, z_0$ ) along the x-axis for angle degrees.
- If Rotate.Y is specified, the cylinder is rotated at position ( $x_0, y_0, z_0$ ) along the y-axis for angle degrees.

## 12: Structure Generation

### Shape Library

If `Rotate.Z` is specified, the cylinder is rotated along the z-axis. The right-hand rule determines the direction of the rotation.

- `angle` is the rotation angle in degrees (see [Figure 126](#)).

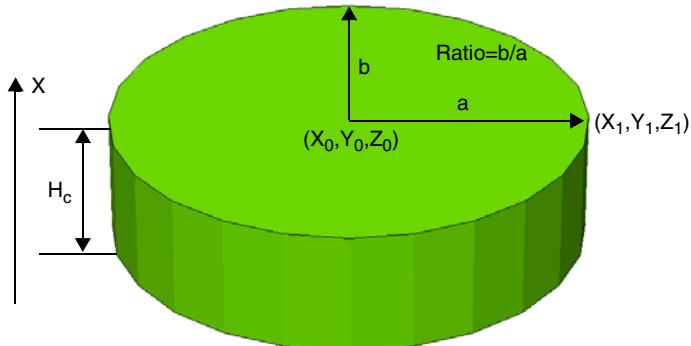


Figure 126 Elliptic cylinder-shaped polyhedron

---

## PolygonSTI

The `PolygonSTI` command creates a 2D STI-shaped polygon. The syntax is the same as for `PolyHedronSTI`, except it does not have the `Zmin` and `Zmax` parameters (see [PolyHedronSTI on page 794](#)).

The syntax is:

```
PolygonSTI name direction X0 Y0 Depth Tsti Asti Hsti Rd Rb Ru [material]
```

where:

- `name` is the name of the polygon.
- `direction` can be `left` or `right` only. This sets the facing direction of the STI polygon.
- `material` is optional and specifies the material of the inserted shape in SDE mode. In MGOALS mode, the material of the inserted shape can be specified using the `insert` command.
- [Figure 119 on page 795](#) describes the other parameters.

## PolygonWaferMask

The `PolygonWaferMask` command creates a wafer mask polygon.

The syntax is:

```
PolygonWaferMask name Y0 Z0 Rw Lf
```

where:

- `name` is the name of the polygon.
- Other parameters give the location and the size of the mask (see [Figure 127](#)).

**NOTE** This command works only in MGOALS mode.

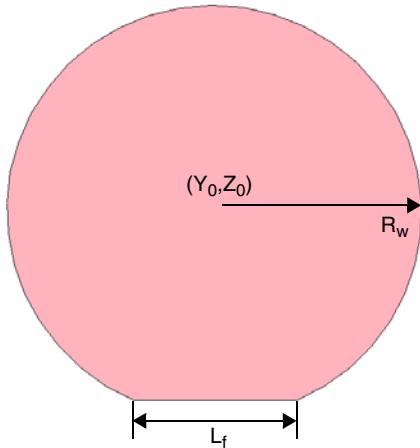


Figure 127 Wafer mask-shaped polygon

## PolyHedronEpiDiamond

The `PolyHedronEpiDiamond` command creates an epitaxial diamond-shaped polyhedron.

The syntax is:

```
PolyHedronEpiDiamond name X0 Y0 Z0 Wepi Lepi Hup Hdown Drcess [material]
```

where:

- `name` is the name of the polyhedron.
- [Figure 128 on page 802](#) describes the other parameters.

## 12: Structure Generation

### Masks and Lithographic Patterning

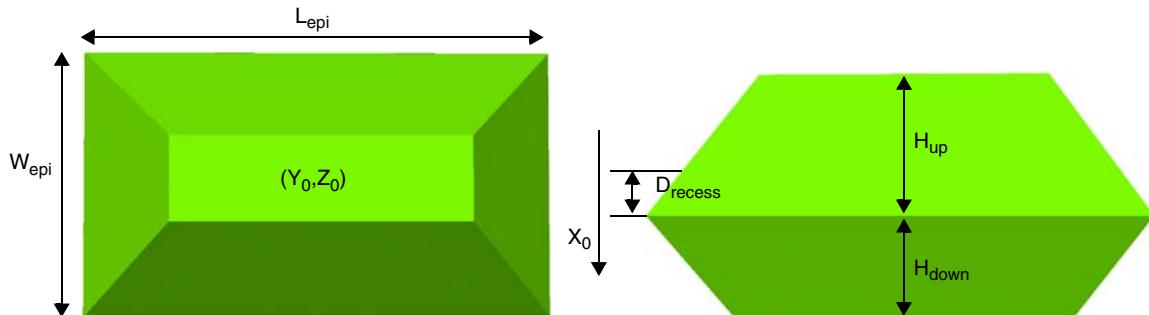


Figure 128 Parameters for generating epitaxial diamond-shaped polyhedron

---

## Masks and Lithographic Patterning

The `photo` command can be used to mimic lithographic patterning. The `photo` command takes a mask and effectively performs a resist spin-on step followed by an exposure bake and etch. The resist layer produced has vertical walls and is a negative of the mask by default, but the positive sense can optionally be created as well.

In addition to the `photo` command, the `etch` and `deposit` commands allow you to use a mask directly. The `mask` argument in the `etch`, `deposit`, and `photo` commands specifies the name of one mask that has been previously defined using a `mask` command or by reading in masks from a layout using the IC WorkBench Edit/View Plus–TCAD Sentaurus interface (see [Chapter 13 on page 835](#)).

The mask will have an effect similar to a masking layer; it limits the etching or deposition process to a certain window. By default, etching is not performed for points inside the mask, unless the `negative` argument is used in the mask definition. Similarly, deposition of a new layer in the `deposit` command and deposition of the photoresist layer in the `photo` command are performed outside the mask unless the `negative` argument is specified in the `mask` command, in which case, deposition occurs inside the mask only.

**NOTE** Always specify the masks and the simulation domain such that masks do not end exactly on the boundary of the simulation domain, but end inside or extend safely beyond the boundary of the simulation domain.

The `mask` command creates a mask. You can define the geometry of the mask directly in the command file or can read masks from a layout file. Masks defined in the command file must be given a name; otherwise, the names are read from the layout file.

If `list` is specified in the `mask` command, information about the existing masks is printed. If `name` is specified as well, information about the specified mask is printed.

If `clear` is specified in the `mask` command, all previous mask definitions are removed. If `name` is specified as well, only the specified mask is removed.

A mask can be defined directly in the command file using different types of geometry object:

- Segments
- Rectangles
- Polygons

Each mask may be composed of an arbitrary number of such objects.

For example, segments are defined as:

```
mask name= pmask segments= { -0.1 0.6 0.7 1.1 }
```

Pairs of subsequent values define the y-coordinates of the beginning and end of one mask segment. Therefore, an even number of coordinates must be specified in the `segments` argument. The pairs may be defined in arbitrary order, and the segments defined by pairs of coordinates may touch or overlap each other. In three dimensions, masks defined by segments are extended over the entire range of z-coordinates.

For example, a rectangular mask is defined as:

```
mask name= nimask left= 0.2 right= 1 front= 0.2 back= 1 negative
```

where:

- `left` and `right` define the minimum and maximum extensions of the mask along the y-axis, respectively.
- `front` and `back` define the minimum and maximum extensions of the mask along the z-axis, respectively.

**NOTE** Only one rectangle can be specified per `mask` command. The `front` and `back` arguments may be omitted; in this case, the mask is equivalent to a mask with one segment. Additional `mask` commands with the same name can be used to add rectangles. The rectangles defined for a mask may arbitrarily intersect or touch each other.

Masks also can be defined by a list of names of polygons. These named polygons must have been defined before the `mask` command using one `polygon` command for each named polygon:

```
polygon name= LShape2 segments= {0.0 -1.5 0.0 -0.5 0.5 -0.5 0.5 1.5 1.5 \
1.5 1.5 -1.5}
mask name= Mask2 polygons= {LShape2} negative
```

## 12: Structure Generation

### Masks and Lithographic Patterning

**NOTE** The segments in the polygon command are defined as a sequence of y- and z-coordinates. The polygon is closed implicitly by connecting the last point to the first. Each polygon for a mask must not touch or intersect itself. The polygon may be specified with arbitrary orientation (clockwise or counterclockwise in the yz plane).

Masks also can be defined by a combination of segments, rectangles, and polygons. Different objects may touch or overlap each other.

In one dimension, the entire simulation domain is masked if the coordinate origin is masked. Any point along the y-axis in a 2D simulation and any point of the yz rectangle of the simulation domain in a 3D simulation are inside the mask if they are contained in any one of the geometry objects defined for the mask. Specifying negative inverts the mask. In other words, any point outside all the geometry objects defined for the mask is *masked*.

Masks can be empty. With an empty mask, the entire simulation domain is unmasked. Correspondingly, with a negative empty mask, the entire simulation domain will be masked.

These commands can be used to invert a mask at any time after it has been defined:

```
mask name=<c> negative  
mask name=<c> !negative
```

**NOTE** In the etch command, the masked area is not etched. While in the photo and deposit commands, the photoresist or the specified material is deposited in the unmasked area.

Masks also can be combined using a set of Boolean operations, which are specified using the bool argument (see [Boolean Masks on page 806](#)).

Layouts that have been defined in the GDSII format can be read into Sentaurus Process using the IC WorkBench Edit/View Plus–TCAD Sentaurus interface (see [Chapter 13 on page 835](#)).

When using a layout, the relation between the layout coordinate system and the Sentaurus Process coordinate system may need to be defined. By default, the layout-x axis corresponds to the Sentaurus Process z-axis. The layout-y axis corresponds to the Sentaurus Process y-axis. This definition matches the default definition of the argument slice.angle of the init command and the coordinate x- and y-axes when displaying the Sentaurus Process simulation results.

The coordinate transformation between the Sentaurus Process coordinate system and the layout coordinate system can be defined in two ways:

- In the mask command that specifies the layout file, the name of one mask may be specified. If a mask with the specified name is contained in the layout file, it is used to position and orientate the simulation domain in the layout.

- Otherwise, a mask with the specified name must have been defined before using a `mask` command. The specified mask is defined in layout coordinates. It may be defined as a rectangle or a polygon, containing at least two points.

In the case of a rectangle defined in a `mask` command, the point with the minimum layout-x and layout-y coordinate is used as the origin of the Sentaurus Process coordinate system. The direction from `(min.layout-x, min.layout-y)` to `(min.layout-x, max.layout-y)` is used as the Sentaurus Process y-axis.

If a polygon of at least two points is used (for example, a mask defined as a polygon), the first point defined is used to place the origin of the Sentaurus Process coordinate system. The direction from the first to the second point of the mask is used as the orientation of the Sentaurus Process y-axis.

The local coordinates of the specified mask with respect to the selected Sentaurus Process y-axis and origin are used as default extensions of the simulation domain. If a polygon mask with only two points is used, the default extension in the z-direction is 0. The default extension in the y-direction is defined by the distance between the two points. The default extensions in the y- and z-directions as defined by the mask are reported. If no extensions have been defined using the `line y` command, or the `line z` command, or both commands, the default extensions are defined for the simulation when the layout file is read.

If a layout file is loaded, but no mask name is specified, the `Cutline2D` command that may have been specified in the `init` command to define the parameter `slice.angle` will be used to orientate the coordinate systems. The first point specified in the `Cutline2D` command is used as the origin of the Sentaurus Process coordinate system. The direction from the first to the second point is chosen as the direction of the Sentaurus Process y-axis. If `Cutline2D` is used, no default extensions of the simulation domain are defined.

---

## Photoresist Masks

To define photoresist layers, use the `photo` command and specify a mask. Sentaurus Process defines photoresist layers by specifying the minimum thickness of the resist and selecting the name of a mask that has been defined by the `mask` command. By default, the photoresist will be deposited outside the specified mask and will have a flat top similar to resist spin-on. If `negative` has been specified when defining the mask, a photoresist is created inside the mask.

## 12: Structure Generation

### Masks and Lithographic Patterning

## Boolean Masks

Two masks can be combined using the `bool` argument of the `mask` command. [Table 93](#) presents the Boolean operations that can be specified in the `bool` argument as well as examples. The `bool` argument only accepts simple expressions.

Complex nested expressions (for example, `bool= "(M1 + M2) - bias(-50, M3 + M4)"`) are not possible. Therefore, they must be reduced to simple operations using a single operator (for example, `bool= "(M1 + M2)"`). Masks requiring a combination of three or more masks must be created using temporary masks to store the intermediate results. In addition, the `bool` argument cannot be used together with `polygon` and `negative`.

Table 93 Boolean operations

Operation	Example	Description
+	<code>bool= "mask1+mask2"</code>	Unites (merges) <code>mask1</code> and <code>mask2</code> .
-	<code>bool= "mask1-mask2"</code>	Subtracts <code>mask2</code> from <code>mask1</code> .  Note that this is a geometric subtraction. Sentaurus Process takes <code>mask1</code> and removes from it the portion of <code>mask2</code> that overlaps <code>mask1</code> . In particular, the operation <code>mask1-mask2</code> is not equivalent to <code>mask1+(-mask2)</code> .
*	<code>bool= "mask1*mask2"</code>	Produces the intersection of <code>mask1</code> and <code>mask2</code> .
^	<code>bool= "mask1^mask2"</code>	Produces a mask that contains the nonoverlapping portions of <code>mask1</code> and <code>mask2</code> (XOR operation).
-	<code>bool= "-mask"</code>	Produces a mask that is the complement of the input mask.
array	<code>bool= "array(nx, ny, dx, dy, mask)"</code>	Produces an array of $n_x \times n_y$ masks separated by a distance specified with <code>dx</code> and <code>dy</code> .
bias	<code>bool= "bias(delta,mask)"</code>	All mask edges on the input mask are offset in the normal direction by the specified amount. A positive <code>delta</code> value expands the mask, while a negative <code>delta</code> shrinks it. Zero or negative area sections of the mask are eliminated from the output mask. Overlapping sections of the mask are merged.
mirror	<code>bool= "mirror(axis,[coordinate,]mask)"</code>	Mirrors a mask with respect to a local axis specified by <code>x</code> or <code>y</code> . The optional parameter <code>coordinate</code> defines the local intercept of the local axis-aligned reference line used for the mirror operation.
offset	<code>bool= "offset(dy, dz, mask)"</code>	Translates the mask by the specified amount. The <code>dz</code> parameter is ignored in two dimensions.

Table 93 Boolean operations

Operation	Example	Description
over_under	bool= "over_under(delta, mask)"	Expands and then shrinks the input mask by <code>delta</code> . This effectively merges areas in close proximity and is equivalent to <code>bias(delta, bias(-delta, mask))</code> .
rotate	bool= "rotate(direction,mask)" bool= "rotate(direction,x0, y0, mask)"	Produces a mask that is rotated with respect to the input mask. The <code>direction</code> parameter can be either <code>left-90</code> or <code>right-90</code> . The optional <code>x0</code> and <code>y0</code> parameters specify the center of rotation. They are specified using the local mask coordinate system. If <code>x0</code> and <code>y0</code> are not specified, the rotation is performed with respect to the center of the bounding box of the mask.
scale	bool= "scale(factor,mask)" bool= "scale(factor,x0, y0, mask)"	Produces a mask that is scaled with respect to the input mask using the floating-point value of <code>factor</code> . The optional <code>x0</code> and <code>y0</code> parameters specify the center of scaling. They are specified using the local mask coordinate system. If <code>x0</code> and <code>y0</code> are not specified, the scaling is performed with respect to the center of the bounding box of the mask.
under_over	bool= "under_over(delta, mask)"	Shrinks and then expands the input mask by <code>delta</code> . This eliminates small areas and is equivalent to <code>bias(delta, bias(-delta, mask))</code> .

---

## Line Edge Roughness Effect

Line edge roughness (LER) is the deviation of feature edges from ideal straight lines due to statistical fluctuations in photolithographic processes. Sentaurus Process uses the `line_edge_roughness` command to apply randomized deviations to straight mask edges, for example:

```
line_edge_roughness normal= "Z" masks= {mask1} correlation.length= 25.00<nm> \
    standard.deviation= 5.00<nm> max.segment.length= 5.00<nm>
```

The random noise function  $f_{\text{random}}$  applied to mask edges by the `line_edge_roughness` command is generated from the power spectrum of a Gaussian autocorrelation function. The Gaussian autocorrelation shape is characterized by the standard deviation distance  $\delta$  specified by the `standard.deviation` argument and the correlation length  $\lambda$ , specified by the `correlation.length` argument:

$$\text{Autocorrelation}(f_{\text{random}}) = \delta^2 \sqrt{\pi} \lambda e^{-(x^2/\lambda^2)} \quad (995)$$

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### Masks and Lithographic Patterning

$f_{\text{random}}$  is obtained by Fourier synthesis, applying the inverse Fourier transform to [Eq. 995](#), after adding random phases. In this way, random deviations of the mask edges can be obtained from run to run, which correspond to LER profiles having the same standard deviation  $\delta$  and correlation length  $\lambda$ .

These random deviations are added in discrete form to the mask edges in question. First, the mask edge is subdivided into discrete segments complying with the `max.segment.length` argument. Second, the deviation at each segment endpoint is added in the direction normal to the initial mask edge orientation.

LER is applied to all edges of the mask by default. You can limit which edges in a named mask receive LER using `normal`, which specifies either the y-axis ("Y") or the z-axis ("Z"). If `normal` is specified, only those edges in the named masks normal to the given axis are chosen for LER to be applied. LER is applied only once per mask. Mask segments along the device bounding box do not receive LER.

The option `!random.reseed` bypasses the reseeding of the random number generator before the random phases are added. Using this option, the shape of the noise function and, therefore, the LER result, can be reproduced from one run to the next if needed for comparison.

The option `random.seed` can reproduce specific LER calculations from one run to the next by setting the same random seed in both runs. When stored in a TDR file in split simulations, `random.seed` is included when saving `line_edge_roughness` to the TDR file, even if it is not specified by users, to ensure proper reproduction of the same LER in a subsequent reload of the TDR file.

**NOTE** The structure is extruded automatically to three dimensions if it is less than three dimensions and the `line_edge_roughness` command is used.

The following strategy is used to address the problem of nearly collinear LER mask points that may trigger removal by decimation during meshing. Avoiding the decimation of nearly collinear LER mask points is desirable because removing such points may perturb the power spectrum of the Gaussian autocorrelation function represented by the mask shape and may also result in meshing difficulties.

If `max.tries` is set to a nonzero value, LER masks are checked for nearly collinear points, which would result in decimation by the mesher:

```
line_edge_roughness max.tries= 30
```

If any points in the LER mask are decimated by the mesher, based on the current `mgoals accuracy=<n>` setting, the LER mask is rejected and the LER generation process is restarted. After each restart, the detection and restart process is repeated until an acceptable LER mask is generated or until the number of attempts exceeds `max.tries`.

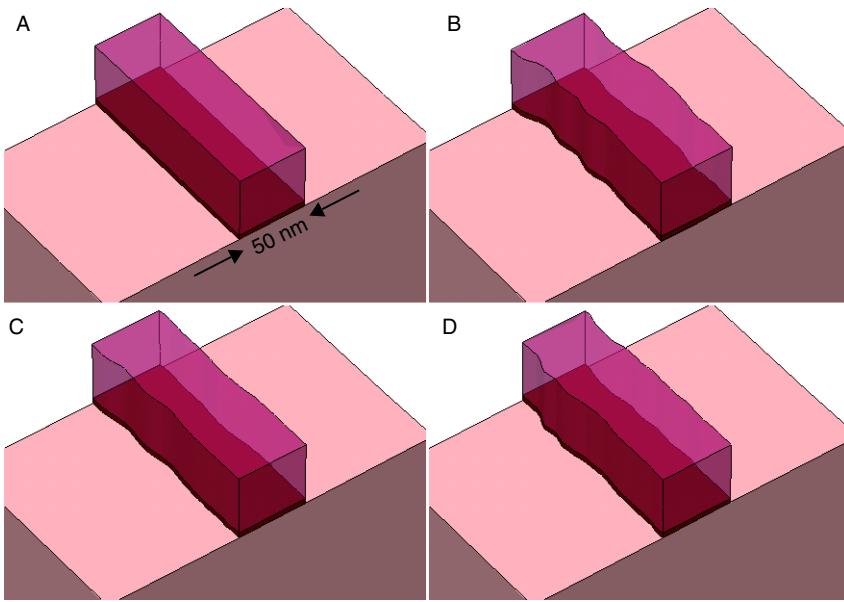


Figure 129 Example of 3D structure with LER applied using different values of standard deviation  $\delta$  and correlation length  $\lambda$ : (A) no LER applied, (B) LER applied with  $\delta = 4 \text{ nm}$  and  $\lambda = 20 \text{ nm}$ , (C) LER applied with  $\delta = 2 \text{ nm}$  and  $\lambda = 20 \text{ nm}$ , and (D) LER applied with  $\delta = 2 \text{ nm}$  and  $\lambda = 12 \text{ nm}$

When `max.tries` is exceeded, Sentaurus Process stops with an error message that suggests using a smaller value of `mgoals accuracy=<n>` or a larger value of `max.segment.length` in the `line_edge_roughness` command.

The default value of `max.tries` is 0, meaning no decimation check is performed, no retries are attempted, and the initial mask LER is accepted as it is, even with nearly collinear points.

## Mirror Boundary Conditions

The addition of LER is inherently 3D and nonsymmetric; therefore, it is not easily compatible as a simulation problem with the assumption of symmetry reduction. Adding LER to a structure reduced by symmetry may produce rough geometric transitions at joined geometric boundaries when pieces are reunited.

To accommodate the possibility of joining symmetry-reduced structures, an additional argument `smooth.points` defines the smoothing of LER at structure boundaries. The default value of `smooth.points` is 0, implying no smoothing.

The use of nonzero `smooth.points` alters the LER function that creates mirror boundary conditions at the structure boundaries. The smoothing occurs at the intersection of masks with the structure boundary sides. The argument `smooth.points` defines the number of segments

in the discrete LER function, counting from the boundary edge of the mask that should be adjusted or smoothed. The length of segments in the discrete LER function is determined using `max.segment.length`.

Smoothing is calculated by generating the LER function, then creating a virtual mirroring at the structure boundary edge where a cubic spline interpolation is applied with a mirror boundary condition. The spline fit is made with the LER at `smooth.points` from the boundary. The smoothed LER function is then applied to the mask.

Applying nonzero values of `smooth.points` affects the randomness and the power spectrum characteristics of the LER offset function at the boundaries as a trade-off for permitting the smooth joining of symmetry-reduced structures.

---

## Geometric Transformations

Transformations supported in Sentaurus Process are reflection, stretch, cut, rotation, translation, and flip:

- The `transform reflect` command is used with `left`, `right`, `front`, or `back` to perform the reflection centered on the outer boundary of the simulation domain. At the reflection side, regions are not merged immediately to allow a clean `transform cut` afterwards if required. The grid can be merged with the `grid merge` command manually, but if not, the structure will naturally be merged for any geometry-changing operation later (except `transform reflect`). It is also possible to discard the original structure when reflecting by specifying `!keep.original`.
- The `transform stretch` command is used to extend the structure. The algorithm cuts the mesh in two pieces using a cutplane defined by `location` and the `left`, `right`, `front`, or `back` arguments. The resulting pieces of mesh are translated perpendicular to the cutplane to create a gap of size `length` in the direction given by `left`, `right`, `front`, or `back`. After this translation, a set of new elements is inserted to connect both sections of the mesh.
- The `transform cut` command crops the structure. The algorithm cuts the structure in two pieces using a cutplane defined by `location` and the `left`, `right`, `front`, or `back` arguments. If `location` is omitted, the algorithm will cut the structure in the middle. The `left`, `right`, `front`, or `back` arguments instruct the algorithm to remove the portion of the structure along the given direction. For a more general crop operation, the `cut` argument can be used with `min` and `max` that specify the cropping box.
- The `transform rotate` command rotates the structure. The `axis` and `angle` arguments must be specified. Only  $90^\circ$ ,  $180^\circ$ , and  $270^\circ$  angles are allowed for the x-axis, and  $180^\circ$  for the y- and z-axis. For 2D simulations, rotations will produce an extruded 3D simulation.
- The `transform translate` command shifts the structure by the specified quantity.

**NOTE** Sentaurus Process KMC does not support the `flip` and `stretch` transformations.

---

## Refinement Handling During Transformation

All transformations apply to the existing refinements created with either the `refinebox` command or the `line` command by default.

To disable this feature, use:

```
pdbSet Grid Transform.Updates.Refinement 0
```

---

## Contact Handling During Transformation

The only special contact handling occurs during `transform reflect`. In this case, contacts that straddle or touch the reflecting plane are enlarged to the reflected area (only one contact remains). The remainder of the contacts are duplicated and are renamed by appending a suffix as follows:

- For right or left reflection, the contact on the left after reflection will be named `<original contact name>.1` (where `<original contact name>` was the name of the contact before the reflection operation), and the contact on the right after reflection will be named `<original contact name>.2`.
- Similarly, for front or back reflection, the front contact (which has a larger z-coordinate) will be named `<original contact name>.2`, and the back contact will be named `<original contact name>.1`.
- For up or down reflection, the upper contact will be named `<original contact name>.1`, and the lower contact will be named `<original contact name>.2`.

You can rename contacts after the `transform reflect` command, or at any time, using the command:

```
contact name=<c> new.name=<c>
```

For example, after reflection, you can use the command:

```
contact name= SourceDrainContact.1 new.name= Source
```

where the original contact name before reflection was `SourceDrainContact`.

**NOTE** It is recommended to specify all contacts *after* all transformation operations other than `transform reflect` to avoid problems during contact creation.

---

## Reflection

The `transform reflect` command reflects the structure about the left, right, front, or back boundary (at minimum y, maximum y, maximum z, or minimum z). If any remeshing or other mesh modification operations are performed after a `transform reflect` command, the symmetry will be lost. Using `!keep.original` discards the original structure leaving only the reflected one.

Examples:

```
transform reflect left
transform reflect ymin
transform reflect front
transform reflect left !keep.original
```

**NOTE** The option `remesh` is disabled in `transform reflect` because it may disrupt the symmetry of the reflected structure. However, the command `grid merge` can be used afterwards to remove same-material interfaces at the reflecting plane.

### Refinement Handling During Reflection

In the case of `!keep.original`, lines coming from both the `line` command and refinement boxes are reflected along with the structure. However, when the original structure is kept, some special handling is required.

Typically, during any geometry operation, lines created with the `line` command that have been defined outside the bounding box will be removed. Therefore, there is no danger of the reflected lines conflicting with the original lines.

For refinements created with refinement boxes, if the refinement box is constrained spatially (that is, `min` or `max` has been used in the definition), the box will be duplicated, and the name of the new box will be `reflected_<c>`, where `<c>` is the name of the original refinement box. If the original and reflected refinement boxes overlap, there is no problem since the refinement criteria are the same.

---

## Stretch

The `transform stretch` command stretches the structure in the left, right, down, up, front, or back directions at a given coordinate location by offsetting one side of the structure by the specified length. If there is no vertical line of edges at the specified location, MGOALS creates

such a line and then stretches the structure. The data at the two ends of the stretched region is exactly the same as that of the unstretched mesh.

Examples:

```
transform stretch location=0.001 length=5 right  
transform stretch down loc=0.5 length=200
```

**NOTE** Do not use together with the atomistic mode (Sentaurus Process KMC).

**NOTE** Do not use a negative stretch length.

## Refinement Handling During Stretch

During the stretch operation, mesh lines that were created with the `line` command in the part of the structure being stretched are translated with the structure. No new lines are introduced into the expanded region. The refinement boxes that straddle the stretch location increase in size by the stretch distance to follow the structure.

---

## Cut

The `transform cut` command cuts at or near the requested coordinate location. The location defines a line in two dimensions, or a plane in three dimensions, that divides the structure into the left and right, or front and back, or up and down parts. You can select the left/right, or front/back, or up/down region to be removed. If a line of element edges in two dimensions, or a plane of element faces in three dimensions, can be identified by MGOALS, the operation eliminates only the elements in the removed region. This works well if a structure had been reflected and needs to be cut back to the original (unreflected) structure. If a line of element edges in two dimensions, or a plane of element faces in three dimensions, cannot be found, a mesh-cutting operation is performed. By default, MGOALS tries to find a mesh line or plane near the specified coordinate. Then, MGOALS removes entire mesh elements rather than cutting mesh elements to avoid arbitrarily small edges and poor element quality.

To disable the search feature and to perform the operation exactly where specified, use `!mesh.align` in the `transform` command, which will invoke a remesh unless `!remesh` also is specified.

Example:

```
transform cut location=0.5 right
```

You also can use the `transform cut` command to crop the mesh by specifying a rectangle or brick defined by the upper-left-front and lower-right-back corners, specified with the `min` and `max` arguments. The cut operation retains the region enclosed by the rectangle or brick. By

default, MGOALS tries to find a mesh line or plane near the specified coordinate and removes entire mesh elements instead of cutting the mesh (which could lead to arbitrarily small edges and poor element quality).

To disable searching of a nearby mesh line or plane, and to perform the operation exactly at the specified location, specify `!mesh.align`, which automatically invokes a remesh unless `!remesh` also is specified.

Example:

```
transform cut min= {-10 1.35 0.15} max= {10 1.65 0.4}
```

## Refinement Handling During Cut

During the cut operation, lines created with the `line` command that are outside of the simulation domain after the cut are removed. Similarly, any refinement box that lies completely outside the simulation domain after the cut is removed as well.

---

## Flip and Backside Processing

The `transform flip` command provides a convenient way to perform process steps on the back of a wafer. During the `transform flip` command, the structure is rotated 180° about a line by default in the center of the structure parallel to the y-axis. Therefore, the structure is upside down after the flip and in the same location.

Because most operations in Sentaurus Process require a gas region on top, a gas region is added automatically. In addition, many meshing operations require a solid material at the bottom of the structure, so the Gas region that was previously on top of the structure is converted to an auxiliary material called `BackMat`. If the structure is flipped again, the reverse happens, namely, `BackMat` is converted to `Gas`, and `Gas` is converted to `BackMat`. Any operation is allowed on a structure that has been flipped one or more times; however, the current bottom of the structure is never an active surface for any operation such as oxidation, epi, etching, and deposition.

There is great flexibility in handling the auxiliary material at the back of the structure. The material itself defaults to `BackMat` as mentioned, but you can choose another material using:

```
pbSet Grid Back.Material <material>
```

The material `BackMat` inherits its parameters from (`is Like`) `Gas` so that it behaves like `gas` for dopant diffusion simulations. For implantation, the material is converted to `Photoresist` so no implantation tables are required for this material. Similarly, for mechanics, the only way to obtain `Gas`-like mechanics boundary conditions at interfaces to the back material is to use an actual `Gas` region. Therefore, the back material is converted automatically to `Gas` before

each mechanics call and is converted back directly afterwards. Finally, when a region of material BackMat is saved in a structure, it is first converted to Gas, so that other tools reading the structure will have the proper material. However, it is also given a tag specific to Sentaurus Process, so that Sentaurus Process knows the region should actually be BackMat.

Another important point regarding mechanics simulations on flipped structures is that only a modified version of the lattice mismatch model is available. With this model, you must not set the location of the top of the relaxed region any more. Instead, the lattice-mismatch strain is added using the reference concentration model. This model uses a reference concentration and bases all strains directly on the difference between the strain field and that reference (see [Reference Concentration Model on page 706](#)).

**NOTE** To avoid switching from the standard lattice mismatch model to the reference concentration lattice mismatch model after `transform flip` is used, switch on the reference concentration model. This should be performed before initial structure creation for those simulations utilizing `transform flip`, using the command:

```
pdbSet Mechanics Reference.Concentration.Model 1
```

**NOTE** When performing laser annealing on a flipped structure, the following settings are recommended (see [Flash or Laser Anneal Model on page 201](#)):

```
pdbSet Grid Zero.Back.Material 0  
mater add name= MyBackMat new.like= Silicon add  
pdbSet Grid Back.Material MyBackMat  
pdbSet ImplantData Back.Material MyBackMat
```

**NOTE** Do not use together with the atomistic mode (Sentaurus Process KMC).

## Refinement Handling During Flip

Refinements during a flip operation are handled in the same way as refinements during reflection in the case of `!keep.original`. Lines coming from both the `line` command and refinement boxes are reflected along with the structure.

---

## Rotation

The `transform rotate` command rotates the structure at the specified angle in the specified axis using (0,0,0) as the rotation center. It accepts two arguments `angle` and `axis` to specify the rotation angle and the rotation axis, respectively. For Y and Z, 180 degrees can be specified. For X, 90, 180, and 270 degrees are allowed.

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### MGOALS

It might happen that, during the rotation, the existing initial gas must be moved to a side or the bottom of the structure instead of being at the top. In these cases, new gas will be added to the top.

The `transform rotate` command applies to 2D and 3D simulations. For 2D simulations, a rotation in the z-axis will produce another 2D simulation. However, rotations in the x-axis and y-axis will produce a structure equivalent to extruding the z-axis and then performing the rotation.

### Refinement Handling During Rotation

During a rotation operation, lines coming from both the `line` command and refinement boxes are rotated along with the structure.

---

## Translation

The `transform translate` command does not change the aspect of the structure. It only adds the coordinate specified in the `translate` argument to all nodes, that is, it displaces the structure or shifts it in space. It is equivalent to changing the origin of coordinates by a fixed quantity.

Similarly, mesh lines created with the `line` command and the bounding box of refinement boxes (which are specified with `min` and `max` of the `refinebox` command) are translated with the structure.

---

## MGOALS

By default, etching and deposition operations are performed using MGOALS in all dimensions. MGOALS operates as follows:

- The starting structure is analyzed for the interfaces that will change during the operation.
- The geometry-changing operations are performed.
- In two dimensions, the entire structure is remeshed. During remeshing, nodes in the silicon region are retained as much as possible in their original locations. In most cases, a high percentage of nodes are retained after remeshing. This minimizes interpolation errors. In three dimensions, the structure is remeshed only if the next step requires an up-to-date mesh.

---

## MGOALS Boundary-Moving Algorithms

MGOALS uses either the analytic method or the fast level-set method to perform boundary-modifying operations. In general, the analytic method is fast, less memory intensive, and more accurate, and uses a simplified string algorithm. However, it cannot handle deposition in concave regions or etching of convex areas when there are boundary collisions and self-intersections.

Due to speed and accuracy advantages, MGOALS always tries to perform an analytic operation. If self-intersections are detected in the new boundary, MGOALS automatically switches from the analytic method to the fast level-set method. Both the analytic method and the fast level-set method can handle simple etching and deposition processes.

Besides the analytic method and the fast level-set method, the general time-stepping level-set method is available to handle more complex etching types such as Fourier, crystallographic, and multimaterial etching, and to include shadowing effects.

Both level-set methods use an approach similar to that described in [1]:

- First, the level-set method identifies the interface or the part of an interface to be moved. This computation is based on nonetched overlayers, masks, and if necessary, visibility due to directional constraints specified by users.
- Second, evolution of the moving interface is performed using either the fast-marching scheme, which solves the time-independent boundary-value formulation of the Hamilton–Jacobi equation (or Eikonal equation), or the *full level-set*, which is a time dependent, initial-value formulation of the same equation. The fast-marching scheme computes the new boundary location for all times in a single step. The nature of the equation is such that it captures and handles collisions. However, the equation cannot identify when the collision actually occurred. The full level-set formulation is used for multimaterial, Fourier, and crystallographic etching, and for handling shadowing effects. Its time-stepping algorithm allows for recalculating the front velocity at every time step.

In MGOALS, the fast-marching scheme and the level-set equations are solved on a separate Cartesian mesh that is independent of the simulation grid. For a description of the parameters that control the Cartesian mesh, see [MGOALS Boundary-Moving Parameters on page 818](#).

After solving the level-set equations, the newly created boundary is extracted from the level-set function on the Cartesian mesh and then incorporated into the simulation mesh. The exact replication of the extracted boundary in the mesh can be expensive and can transfer unwanted noise from the level-set solution into the structure. To resolve these issues, MGOALS allows a certain smoothing to be performed on the extracted boundary.

In two dimensions, to incorporate the new boundary into the simulation grid, a simplified meshing step is performed. A simple mesh is created for the modified regions and connected

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### MGOALS

to the mesh in unchanged regions. Since this mesh is not suitable for process simulation, by default, a full remesh is performed after each etching and deposition step.

In three dimensions, almost all boundary-modifying operations performed by MGOALS use the analytic method. The only exceptions are isotropic deposition and etching, which are performed using the fast level-set method. The new material boundary is integrated into the structure using a set of polyhedral Boolean operations.

## MGOALS Boundary-Moving Parameters

Parameters to specify the resolution of the Cartesian mesh and the interface fidelity are defined in an `mgoals` command before the `etch` or `deposit` command. These parameters are applied to the entire structure. The interface quality and resolution are controlled by `accuracy`, `resolution`, and `full.resolution`. The actual size and the placement of the Cartesian mesh bounding box is calculated starting with the initial interface being etched, extended based on the time and rates given by the user, or in the case of etch stops, extended based on the distance from the initial front to the etch stops.

### The accuracy Argument

The `accuracy` argument controls the noise and features at an interface. A small value of `accuracy` allows only small deviations between the boundary extracted from the level-set method and the piecewise linear segments incorporated into the simulation mesh. As a result, a large number of small segments may be created. In addition, a value of `accuracy` that is too small may *interpret* numeric noise as surface features, which MGOALS requires to reproduce in the simulation mesh. The default value and unit for `accuracy` is  $1.0 \times 10^{-5} \mu\text{m}$ .

**NOTE** The default value for `accuracy` works well for small structures that are approximately  $1 \mu\text{m} \times 1 \mu\text{m}$  in size. For larger structures, you can scale up this argument to reduce geometric noise. However, using too large a value could lead to self-intersection around sharp features, to meshing failure, and to noticeable loss of curvature in rounded areas.

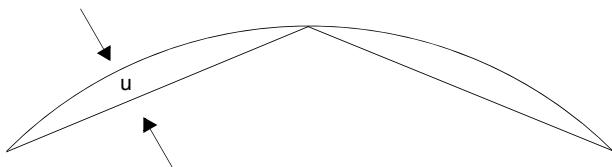


Figure 130 The curved surface represents the extracted new boundary and the piecewise linear segments represent the simplified boundary incorporated into the simulation mesh; the `accuracy` argument ensures that  $u \leq \text{accuracy}$

## The resolution Argument

The value of the `resolution` argument controls the element size in the Cartesian mesh used to perform level set-based etching and deposition. Since the thickness of the layer to be deposited or etched is user specified, the grid size is defined as a fraction of the thickness of the modified layer. The size of each grid element of the level-set mesh is given by the product of the value of `resolution` and the etching or deposition thickness.

The `resolution` is specified in the `mgoals` command, and the etching or deposition thickness is specified in the `etch` or `deposit` command, respectively. This scheme usually provides a good approximation of the required level-set resolution and is computationally efficient. The default value for `resolution` is 0.1.

**NOTE** Providing a small `resolution` for thin layers may lead to excessive time and memory consumption. For example, an isotropic deposition of 1 nm thickness with `resolution=0.1` will result in facets of approximately 1 Å in size. In this case, `resolution=0.3` would lead to coarser facets in rounded areas.

**NOTE** For a thick etching or deposition, it may be necessary to reduce `resolution`. For example, `resolution=0.1` for a 1 μm deposition leads to a level-set grid size of 100 nm, which may lead to a poor approximation of sharp corners and rounded areas in the new boundary.

**NOTE** It is not recommended to set the `resolution` argument to a value greater than 0.3. Doing so may compromise the integrity of the layers being deposited or etched, since they may not be resolved by the level-set grid.

## General Time-Stepping Level-Set Parameters

The general time-stepping level-set method has some additional parameters to control and balance accuracy, simulation time, and memory use.

Usually, the full time-stepping level-set method is used in situations where more intricate boundaries will be generated. This method is needed for Fourier, crystallographic, and multimaterial etching, and for etching with shadowing. It is also used if the option `force.full.levelset` is specified.

The `full.resolution` argument can be used for the time-stepping level-set method in the same way `resolution` is used for the fast level-set method. You also can specify the actual spacing of the Cartesian mesh in the x-direction, or y-direction, or both directions, with the `dx` and `dy` arguments (and the z-direction in three dimensions with `dz`). Reducing the mesh size causes the time-stepping level-set method to allocate more memory, to take smaller time steps, and to increase the solve time for each time step, thereby increasing the overall simulation time.

**NOTE** In previous releases, the *Upwind* formulation of the time-stepping level-set method provided users with the arguments `reinitfrequency` and `reinititerations` of the `mgoals` command to control the frequency and quality of level-set reinitialization. The currently implemented Lax–Friedrichs formulation does not provide these parameters to users, since reinitialization is performed at each time step.

### Level-Set Cartesian Mesh and Resolution: Internal Calculations

The Cartesian mesh extent or bounding box, the `resolution` and `full.resolution` criteria, and the grid spacing criteria `dx`, `dy`, and `dz` interplay in the following ways.

The Cartesian mesh encompasses the initial interface between the Gas and all the materials the user has defined to be etched. It also encompasses the entire movement of the etching front expected throughout the entire etching process. In the case of time-based etching with the `time` argument, an etching distance is computed, based on the requested etching time multiplied by the maximum expected etching rate. The `resolution` or `full.resolution` argument is then used as the approximate mesh spacing unless overridden by `dx`, `dy`, or `dz`. The number of resulting Cartesian mesh lines follows as required to achieve the required mesh spacing within the Cartesian mesh bounding box.

In the case of an etch stop, the bounding box of the Cartesian mesh is calculated based on the initial gas–etching material interface, and its extent is determined by the position of etch stops in the simulation domain, that is, the estimated maximum etching distance. The target mesh spacing in two dimensions is the `resolution` or `full.resolution` multiplied by the estimated maximum etching distance. In three dimensions, the target mesh spacing is set to `min.levelset.size`, because the estimated maximum etching distance is not calculated in three dimensions for this purpose. From the size of the Cartesian mesh bounding box and the target mesh spacing, possibly overridden by `dx`, `dy`, and `dz`, the number of Cartesian mesh lines is determined.

### Limitations of Level Set

As a general approach, while the level-set method is especially useful for shadowing, multimaterial, sophisticated etch velocity functions (for example, surface normal dependent or crystal direction dependent), and for complex evolution of etch surfaces (that is, complicated structures), it is generally not a good choice when sharp or exact corners, and straight or exact etch walls, are required, such as in anisotropic etching.

This limitation is due to the implicit representation of the structure as a rectilinear grid of distance functions used to calculate the evolution of the moving surfaces.

---

## MGOALS 3D Boundary-Moving Algorithms

In three dimensions, a combination of level set, fast marching, and analytic techniques are used to perform geometric operations similar to the 2D mode. In three dimensions, MGOALS can reliably handle complicated polyhedral boundaries. This mode can perform any of the geometric operations contained in the deposit, etch, photo, polyhedron, and transform commands.

**NOTE** After any one of these process steps is performed in three dimensions, all subsequent geometric operations should be performed using MGOALS.

The use of the level-set method for thin etches or deposits can be prohibitively CPU intensive and memory intensive, especially for large structures or for very thin etching or deposition steps. To address this issue, etches and deposits less than 1 nm use the analytic method by default. The thickness of this cutoff can be modified using analytic.thickness of the mgoals command.

To produce meshes with the highest quality elements and the fewest points, you should reduce the number of interfaces in the structure. This is especially true for 3D simulations.

**NOTE** When the command sde off is specified, region-merging is switched on regardless of the previous setting.

---

## Summary of MGOALS Etching

[Table 94 on page 822](#) summarizes the methods used internally to implement etching:

- Level set (LF) – General time-stepping level-set method with Lax–Friedrichs formulation.  
This is the most general method. All level-set methods have the disadvantage of a certain amount of rounding at corners and edges. The LF formulation has added stability, which can result in slightly more rounding at corners and edges.
- Fastmarch – The fast level-set method is used in simple 1D or 2D directional and anisotropic etching.
- Geometric – Three-dimensional etching algorithm inserts an analytically calculated etching shape into the device structure.
- Analytic – One-dimensional or 2D etching algorithm calculates and inserts an analytically calculated etching shape into the device structure.

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### MGOALS

Table 94 Summary of etching algorithms used for different etching input parameters

Material	Shadowing	Etching type	Structure dimension	Etchstop mechanism		
				Time and rate	Material Etchstop	Thickness
Single material	No shadowing	Isotropic	1D	Analytic	Level set (LF)	Analytic
			2D	Fastmarch	Level set (LF)	Fastmarch
			3D	Geometric	Level set (LF)	Geometric
		Fourier	1D/2D/3D	Level set (LF)	Level set (LF)	Not supported
		Directional	1D/2D	Analytic	Analytic	Analytic
			3D	Geometric	Level set (LF)	Geometric
	Shadowing	Anisotropic	1D/2D	Analytic	Analytic	Analytic
			3D	Geometric	Level set (LF)	Geometric
		Isotropic	2D	Level set (LF)	Level set (LF)	Level set (LF)
			3D	Level set (LF)	Level set (LF)	Level set (LF)
			Fourier	2D/3D	Level set (LF)	Level set (LF)
		Directional	2D/3D	Level set (LF)	Level set (LF)	Level set (LF)
		Anisotropic	2D/3D	Level set (LF)	Level set (LF)	Level set (LF)
Multimaterial	No shadowing	Isotropic	2D	Level set (LF)	Level set (LF)	Fastmarch
			3D	Level set (LF)	Level set (LF)	Geometric
		Fourier	2D/3D	Level set (LF)	Level set (LF)	Not supported
		Directional	2D	Level set (LF)	Analytic	Analytic
			3D	Level set (LF)	Level set (LF)	Geometric
		Anisotropic	2D	Level set (LF)	Analytic	Analytic
			3D	Level set (LF)	Level set (LF)	Geometric
	Shadowing	Isotropic	2D	Level set (LF)	Level set (LF)	Level set (LF)
			3D	Level set (LF)	Level set (LF)	Geometric
		Fourier	2D/3D	Level set (LF)	Level set (LF)	Not supported
		Directional	2D	Level set (LF)	Level set (LF)	Level set (LF)
			3D	Level set (LF)	Level set (LF)	Geometric
		Anisotropic	2D	Level set (LF)	Level set (LF)	Level set (LF)
			3D	Level set (LF)	Level set (LF)	Geometric

---

## MGOALS Backward Compatibility

Default parameters and algorithm settings used by MGOALS can change from release to release in the pursuit of more accurate, more realistic, and more stable structure generation results. To use the default parameters and settings from a previous release, type the required release as a string in the `mgoals` command, for example:

```
mgoals "M-2016.12-SP1"
```

Partial support for this backward compatibility is available starting with Version D-2010.03 with more complete support starting with Version E-2010.12.

---

## Boundary Repair Algorithm

Anisotropic or directional operations can produce residual material when the walls of the etched material are not perfectly vertical or aligned to the etching beam. These residual materials usually cause problems for the mesh generator since they contain sharp angles and small features that cannot be meshed. To correct this problem, the boundary repair algorithm can analyze the structure and eliminate small unwanted features.

The boundary repair algorithm can be used with the `deposit`, `etch`, and `photo` commands. These commands include the `repair` option that controls this algorithm. The boundary repair algorithm is enabled by default in 3D and disabled in 2D.

To activate or deactivate the boundary repair algorithm, include `repair` or `!repair` in the command specification, for example:

```
etch material= {Silicon} anisotropic rate= 0.001 time= 1.0 !repair
```

The repair algorithm also can be controlled globally for the `etch` and `deposit` commands. To disable or enable repairs, use the following options in the `mgoals` command (see [mgoals on page 1083](#)):

- `repair.2d`, `repair.2d.deposit`, `repair.2d.etch`, `repair.2d.photo`
- `repair.3d`, `repair.3d.deposit`, `repair.3d.etch`, `repair.3d.photo`

---

## Structure Assembly in MGOALS Mode

Sentaurus Process can read a 2D or 3D structure from a file and paste it into the current 2D or 3D simulation, respectively.

## 12: Structure Generation

### MGOALS

To perform structure assembly, use:

```
paste (direction= back | front | left | right) tdr=<c>
```

where:

- In two dimensions, direction can be `left` or `right`.
- In three dimensions, direction can be `back`, `front`, `left`, or `right`.
- `tdr` specifies the TDR file from which a structure will be read and pasted into a simulation.

Sentaurus Process automatically shifts the structure read from the file to the appropriate quantity in `x`, `y`, and `z` to fit to the current structure. Nevertheless, Sentaurus Process will not automatically stretch the incoming structure. Consequently, for the operation to succeed, the sizes of the pasting planes of the incoming structure and the existing one must be the same.

The values of the fields are conserved for each structure and are interpolated at the interface between the structures.

**NOTE** Structure assembly requires that the structure read from the file must have the same dimensionality, 2D or 3D, as the existing structure.

**NOTE** In three dimensions, structure assembly must be performed in MGOALS mode. That is, structure assembly is not available when `sde on` is specified.

---

## Multithreading

Some of the more sophisticated etching and deposition types require the use of the level-set method (such as multimaterial etching, crystallographic etching and deposition, and Fourier etching and deposition). This can be time consuming, especially for 3D summations. To minimize simulation time, MGOALS allows for a multithreaded solution of the level-set equations.

The multithreaded operation can be invoked using:

```
math numThreads=<i>
```

or:

```
math numThreadsMGoals=<i>
```

where `<i>` is an integer. It is suggested to keep `<i>` at or below 4 to obtain reliable speed improvement.

---

## Insertion: Internal Mode

This section describes different insertion operations.

---

### Inserting Segments

The `insert` command defines and inserts regions defined by segments in one dimension (see [insert on page 1024](#)). You can choose which materials or regions are replaced, and the name and the material of the new region.

Multiple regions can be inserted in one step. However, to insert multiple regions, the name cannot be specified. If multiple regions are inserted, machine-generated names are used.

---

### Inserting Polygons

Two-dimensional regions defined by polygons can be created and inserted directly into a 2D simulation.

Polygons are created with the `polygon` command, which accepts several arguments to specify how to create the polygon:

- `points` specifies a list of points defining the polygon.
- `rectangle`, with `min` and `max`, specifies the rectangle limits.
- `segments` specifies pairs of numbers, which are the coordinates where each segment starts and the previous one finishes.
- `xy` specifies the polygon will be created in the `xy` plane.

Since the standard use of the `polygon` command (see [Masks and Lithographic Patterning on page 802](#)) is to create masks for the `deposit`, `etch`, and `photo` commands, the default coordinates are `y` and `z` for the `segments` and `min` and `max` arguments. Consequently, the option `xy` must be specified in order for the polygon to be created in the `xy` plane instead of the `yz` plane.

- `tdr` specifies the name of a TDR file from which to import the polygon, and the argument `materials` specifies the material or list of materials that will be read from the TDR file specified.

The `insert` command takes the mandatory `polygon` argument that specifies the name of the polygon and inserts it into the structure. It allows you to specify the `replace.materials`, `new.material`, `replace.regions`, and `new.region` arguments in a very similar way to the insertion in three dimensions (see [Inserting Polyhedra on page 828](#)).

## Inserting Polyhedra

Regions defined by polyhedra can be inserted into 3D structures. The `polyhedron` command creates a polyhedron and adds it to the internal polyhedron list.

You can build a polyhedron in different ways. However, only one of them can be used at a time in one `polyhedron` command (see [polyhedron on page 1128](#)):

- Reading polyhedra from a TDR boundary file.
- Creating a cuboid (brick) polyhedron.
- Extruding a 2D polygon in the x-dimension.
- Creating a polyhedron from the beginning using its constituent polygonal faces `<pol1>` to `<poln>`.

### Reading Polyhedra From TDR Boundary File

To read all the polyhedra included in a TDR boundary file called `<c>`, use the command:

```
polyhedron name=<c> tdr=<c> [materials= {<mat1> ...<matn>}]
[regions= {<reg1> ...<regn>}]
```

The optional argument `materials` specifies which materials are included. In addition to explicit material names, you can use `materials=bulk.materials` to specify all nongaseous materials.

The optional argument `regions` specifies which regions of the boundary are included.

If neither `regions` nor `materials` is specified, all regions are assumed to be included. If both `regions` and `materials` are specified, the union of the two is assumed.

Several polyhedra can be included in a TDR file. Any valid TDR boundary file is allowed, regardless of the tool used to create it.

### Creating a Cuboid (Brick) Polyhedron

To create a cuboid polyhedron given the coordinates of two diametrically opposite corners, use the command:

```
polyhedron name=<c> brick= {<minx> <miny> <minz> <maxx> <maxy> <maxz>}
```

## Extruding 2D Polygons

To take a 2D polygon (created with the `polygon` command) and to extrude it in the x-direction from `min` to `max` to build a 3D polyhedron, use the command:

```
polyhedron name=<c> polygons= <list> min=<n> max=<n>
```

The command expects the polygon to be planar. Only one polygon name is expected in the `polygons` list.

## Creating Polyhedron From Its Constituent Polygonal Faces

To build a polyhedron given its definition as a set of polygons, use the command:

```
polyhedron name=<c> polygons= {<pol1> <pol2> ... <poln>}
```

The polygons are `<pol1>` to `<poln>`. Obviously, the command expects the polygon list to form a valid polyhedron, that is, a compact, enclosed, nonintersecting 3D space. The polygons can be created with the `polygon` command.

---

## Insertion: External Mode

This mode differs from the standard Sentaurus Structure Editor mode (see [Sentaurus Structure Editor Interface on page 829](#)) in that a structure can be created inside Sentaurus Structure Editor independently of the existing Sentaurus Process structure. The minimum syntax needed for creating an external structure is:

```
sde external {<Sentaurus Structure Editor commands>}
```

where `<Sentaurus Structure Editor commands>` are Scheme commands that are sent directly to Sentaurus Structure Editor. As an option, a polyhedron can be specified to initialize the structure, and after `sde external`, further geometric commands such as `etch`, `deposit`, and `transform` operate on the external structure until the command `sde off` is specified. See [sde on page 1165](#).

To create a polyhedron from an external structure, the option `external.sde` of the `polyhedron` command must be given. In the following example, an aluminum sphere is inserted into a Sentaurus Process structure:

```
math coord.ucs
sde external {
    (sdegeo:create-sphere (position 0.4 0.0 0.0) 0.9 "Aluminum" "Aluminum_1")
}
polyhedron name= sphere external.sde
```

## 12: Structure Generation

### Insertion: External Mode

```
sde off  
insert polyhedron= sphere
```

---

## Inserting Polyhedra

The `insert` command is:

```
insert polyhedron=<c> [replace.materials= {<mat1> <mat2> ...<matn>}]  
[replace.regions= {<reg1> <reg2>...<reg2>}] [new.material=<c>]  
[new.region=<c>]
```

**NOTE** The argument `polyhedron` is mandatory and specifies the name of the polyhedron with which to operate. This polyhedron must have been previously defined with the `polyhedron` command (see [Inserting Polyhedra on page 826](#)).

The optional argument `replace.materials` lists the materials to be replaced by the polyhedron. In addition to explicit material names, you can use `replace.materials=bulk.materials`. If `replace.materials=bulk.materials` is specified, all materials in the structure, except gas, will be replaced.

The optional argument `replace.regions` lists the regions to be replaced by the polyhedron. If neither `replace.regions` nor `replace.materials` is specified, all materials are replaced. If both `replace.regions` and `replace.materials` are specified, the union of the two is assumed.

If the optional argument `new.material` is specified, all the regions in the polyhedron will change to the specified material. This argument does not change the polyhedron information except temporarily for the duration of the `insert` command. The material name in the inserted polyhedron is inserted, but not in the original polyhedron.

The optional argument `new.region` is valid only when there is one region. When set, the region name is set to the specified one after insertion. The region name in the inserted polyhedron is affected, but not the original polyhedron.

The `insert` command can perform *Polyhedron etching* and *Polyhedron deposition* as well as more general polyhedron insertion. Polyhedron etching is performed by specifying `new.material=gas` in the `insert` command or by creating a gas polyhedron. Polyhedron deposition is performed by specifying `replace.materials=gas` in the `insert` command as well as choosing one or more bulk regions or materials in the `Polyhedron` command, such as `materials=bulk.materials` or `new.material=Silicon`.

**NOTE** The boundaries of the polyhedra to be inserted must not overlap any interfaces or outer boundaries of the structure. Otherwise, it is likely the operation will fail.

---

## Sentaurus Structure Editor Interface

Sentaurus Structure Editor can perform 3D etching, deposition, and geometric transformation operations. It uses the ACIS solid geometry modeling kernel and the Scheme scripting language. Structures are created using CAD operations and process emulation operations. All `3D etch`, `deposit`, `strip`, `photo`, `mask`, and `transform` commands are translated into appropriate Scheme commands that are then dispatched to Sentaurus Structure Editor.

Sentaurus Process provides an interface to Sentaurus Structure Editor.

Sentaurus Structure Editor also can be used as a standalone tool to build the final structure using both its user interface and scripting capability. Then, the final structure can be used in Sentaurus Process either as a boundary file or after remeshing the structure. The mesh or the boundary for the final structure is loaded and, before each implantation or diffusion step, the material of all regions, not yet present in the structure for the process step, is changed to gas.

In addition, the Sentaurus Structure Editor external mode allows independent (that is, external) structures built in Sentaurus Structure Editor to be inserted into structures created with MGOALS (see [Insertion: External Mode on page 827](#)).

Hereafter, the standard Sentaurus Structure Editor mode (`sde on`) is referred to as the *SDE mode*.

As usual, simulations may start in one or two dimensions. If a 3D mask is encountered and if z-lines have been defined, the structure will be extruded to three dimensions, and if the SDE mode is switched on, the Sentaurus Structure Editor interface will be initialized. All subsequent structure-modifying steps in the `etch`, `deposit`, `strip`, `photo`, and `transform` commands are dispatched to Sentaurus Structure Editor.

**NOTE** Reading a discretized 3D structure in Sentaurus Structure Editor can be unstable. Most isotropic operations (deposition or etching) will fail if this method to initialize Sentaurus Structure Editor is used. Therefore, when initializing a 3D simulation, you should store and load .sat files, rather than simply loading a 3D TDR boundary or grid file.

When the 3D structure has been initialized in Sentaurus Structure Editor, structure generation commands (`mask`, `etch`, `deposit`, `photo`, `strip`, and `transform`) are translated by Sentaurus Process into appropriate Scheme commands and then dispatched to Sentaurus Structure Editor.

**NOTE** Some arguments of the `etch` command cannot be translated into appropriate Scheme constructs: Fourier etching, trapezoidal etching, crystallographic etching, and shadowing effects are not supported in three dimensions. The argument `etchstop` only works with CMP not with other etching types.

The modified structure will be retrieved from Sentaurus Structure Editor and remeshed when a command that requires the geometry and the mesh to be synchronized (for example, `implant`, `diffuse`, and `struct` commands that write the mesh to a file) is found in the Sentaurus Process command file.

This ‘lazy’ remeshing (only when needed) minimizes the number of 3D remeshing operations and, therefore, increases both the robustness and speed of the 3D structure generation and remeshing.

The `sde` command is used to configure and control the Sentaurus Structure Editor interface and to specify Scheme commands directly (see [sde on page 1165](#)).

You must specified the following command in each 3D simulation so that the simulation is performed using the Sentaurus Structure Editor interface:

```
sde on
```

To switch off the SDE mode, use:

```
sde off
```

The argument `logfile` of the `sde` command specifies a file name in which to record all Scheme commands that are dispatched to Sentaurus Structure Editor. At the end of the simulation, a complete Scheme script is generated that can be used in a standalone run for debugging, testing different algorithms, or fine-tuning a few command parameters for Sentaurus Structure Editor without rerunning the Sentaurus Process simulation, for example:

```
sde -l logfile.scm
```

These modified parameters and algorithm selections can later be incorporated into the `etch`, `deposit`, and other commands by specifying the argument `sde` in these commands:

```
deposit oxide thickness= 5<n m> isotropic \
    sde= {"algorithm" "lopx" "adaptive" #t "radius" 0.075}

etch silicon thickness= 0.2<um> isotropic \
    sde= {"algorithm" "lopx" "radius" 0.07 "vexity" "convex" \
        "blend-global" "steps" 1 "overetch" 0.2}

deposit oxide thickness= 5<n m> isotropic sde= {"algorithm" "lopx"}
```

**NOTE** The Scheme language is incompatible with the Tcl used by Sentaurus Process. Therefore, all Scheme commands and parameter settings must be enclosed by a pair of braces. The opening brace must be on the same line as the `sde` argument.

In the `sde` command, the braces can contain any number of Scheme commands, each of which starts on a new line.

Since the braces protect the Scheme commands and parameter settings from being parsed by Tcl, they must not contain any calls to Tcl procedures in Tcl expressions. The Scheme language provides its own set of expressions, parameter definitions, and other language constructs.

You should increase the default verbosity level when working with the `sde` command:

```
pdbSet InfoDefault 1
```

Sentaurus Structure Editor does not provide any error-processing facility for errors that have occurred during the solid modeling operations. This can be time consuming if a structure generation step fails and a long `diffuse` or `implant` simulation is performed for an incorrect structure. To avoid this, use a few runs with the `-f` command-line option to adjust the commands and to verify that the proper structure is created. In addition, by default, all boundary files that are written in `struct` commands in the fast mode and before remeshing are read and checked for any geometric inconsistencies. If any defects are observed, the simulation is stopped with an error. To prevent this checking, specify `!SdeCheck`.

**NOTE** By default, Sentaurus Process performs stress relaxation at the end of each etching and deposition step. This requires that a boundary-fitted mesh be constructed at the end of each step. If you do not want to track the stress through all the process steps, use the following command before starting 3D structure generation:

```
pdbSet Mechanics EtchDepoRelax 0
```

**NOTE** To prevent adjacent regions of the same material (for example, gas regions) from merging, switch off region-merging using the command `pdbSet Grid No3DMerge 1`. During the process, as more regions need to be considered (for example, nitride spacer), appropriate materials must be reverted from gas to the required materials.

The option `Grid Auto3DMergeAndSeparate` (off by default) adds the following commands at the end of `photo` and `depo` when switched on:

```
(sdegeo:bool-unite (find-material-id 'depositedMaterial'))  
(sde:separate-lumps)
```

Only the second command is added after etching.

---

## Sentaurus Topography Interface

Sentaurus Process provides an interface to Sentaurus Topography, which is a 2D physical etching and deposition simulator.

Each `sptopo` command first transfers the current 2D geometry from Sentaurus Process to Sentaurus Topography. Then, it dispatches the command to Sentaurus Topography. Finally, it retrieves the modified 2D geometry from Sentaurus Topography and creates a mesh for it.

Sending a new geometry from Sentaurus Process to Sentaurus Topography has been restricted to cases where the geometry has actually been modified in Sentaurus Process after last retrieving the structure from Sentaurus Topography, for example, when using the Sentaurus Process `etch` or `deposit` command. Provisions also are made to detect whether Sentaurus Topography has actually modified the structure or simply a definition of it, for example, a new machine has been added to Sentaurus Topography. Remeshing is restricted to the commands that actually have changed the structure.

During syntax checking, Sentaurus Topography commands are dispatched to Sentaurus Topography and are checked for syntactical correctness. The syntax of the `sptopo` command is (see [sptopo on page 1206](#)):

```
sptopo <Sentaurus Topography command>
sptopo {<Sentaurus Topography command>
         <Sentaurus Topography command>
         ...
}
```

or:

```
sptopo {
    <Sentaurus Topography command>
    <Sentaurus Topography command>
    ...
}
```

The first form of the `sptopo` command allows use of all the usual Sentaurus Process Tcl constructions in the parameter specifications of `<Sentaurus Topography command>`. This form of the command is parsed through the Tcl interpreter. Otherwise, the syntax used for the `<Sentaurus Topography command>` is the same as in each of the commands for a standalone Sentaurus Topography run. In Sentaurus Process command files, each Sentaurus Topography command must start with `sptopo`.

In the second form of the command, the pair of braces prevents the Sentaurus Topography commands from being parsed by the Tcl interpreter. No Tcl expressions must be used in this form of the `sptopo` command. On the other hand, any number of Sentaurus Topography commands can be provided in the second form of the command, each on a separate command line. If necessary, the structure will be sent from Sentaurus Process to Sentaurus Topography

once at the beginning, and retrieved and remeshed once at the end of the entire command sequence.

### **Example 1**

The following command performs two planar deposition steps in Sentaurus Topography, where the first step fills the structure with oxide up to 5 nm above the top material position, and the second step adds a planar layer of 180 nm polysilicon:

```
sptopo {  
    deposit material= Oxide thickness= 0.005  
    deposit material= PolySilicon thickness= 0.180  
}
```

The structure is sent to Sentaurus Topography once, retrieved, and remeshed once at the end of both deposition steps.

### **Example 2**

If masks are required in a Sentaurus Topography simulation, segments can be specified in the sptopo command as shown here. Alternatively, you can use the Sentaurus Process photo command with a mask to define a photoresist layer that will protect certain areas from being etched in an sptopo etch command.

The Sentaurus Process strip command, or the following sptopo command, can be used later to remove the entire photoresist layer:

```
sptopo etch material=Photoresist complete
```

### **Example 3**

The following example defines a mask in Sentaurus Topography including:

- Geometric etching of polysilicon, which is strictly vertical and restricted to the outside of the specified mask segments.
- An anisotropic etching machine.
- Execution of an anisotropic oxide etching in Sentaurus Topography.

```
sptopo {  
    mask name=m1 s0=-1.1 e0=-0.3 s1=0.3 e1=1.1  
    etch material=PolySilicon depth=0.185 mask=m1  
  
    machetch name=oxe1 material=Oxide anisotropy=1 rate=1  
    etch machname=oxe1 time= 0.02 dx=0.03 dy=0.03 mask=m1  
}
```

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### Sentaurus Topography 3D Interface

To increase the default verbosity level when working with the `sptopo` command, use:

```
 pdbSet InfoDefault 1
```

For details about the commands, parameters, and syntax rules of Sentaurus Topography, refer to the *Sentaurus™ Topography User Guide*.

---

## Sentaurus Topography 3D Interface

Sentaurus Process provides an interface to Sentaurus Topography 3D, which is a three-dimensional physical etching and deposition simulator.

The Sentaurus Topography 3D interface makes advanced etching and deposition models of Sentaurus Topography 3D available from within Sentaurus Process.

The subset of 3D commands that are needed for etching and deposition is available through the interface. The `topo` command in Sentaurus Process enables all the interface functionality (see [topo on page 1235](#)). The `topo` command is followed by the respective Sentaurus Topography 3D commands:

```
 topo {<Sentaurus Topography 3D commands>}
```

For a list of the supported Sentaurus Topography 3D commands, refer to the *Sentaurus™ Topography 3D User Guide*.

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## References

- [1] J. A. Sethian, *Level Set Methods and Fast Marching Methods: Evolving interfaces in computational geometry, fluid mechanics, computer vision, and materials science*, Cambridge: Cambridge University Press, 1999.

# ICWBEV Plus Interface for Layout-Driven Simulations

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*This chapter describes how to use the IC WorkBench Edit/View Plus–TCAD Sentaurus interface.*

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## Overview

The IC WorkBench Edit/View Plus (ICWBEV Plus)–TCAD Sentaurus interface drives the TCAD simulations from the GDSII or OASIS layout file provided by designers, which could be at any level of integration in the hierarchy: full chip, test chip, or a single cell.

The TCAD simulation domain can be conveniently chosen using specific markups in the layout file. A single process flow can be defined for all devices in the layout and can be applied easily with minimal adjustments for 1D, 2D, and 3D simulation domains. For meshing, it provides the unique feature of layout-driven meshing. Electrical contacts can be defined easily using auxiliary masks.

This chapter includes the following sections:

- [Introducing ICWBEV Plus for TCAD Users on page 836](#) provides basic ICWBEV Plus training, especially with relevance to TCAD.
- [Sentaurus Markup Files and TCAD Layout Files on page 847](#) introduces the files and file formats used in the ICWBEV Plus–TCAD Sentaurus interface.
- [Starting ICWBEV Plus in Batch Mode and Using Macros on page 854](#) introduces working with macros and running ICWBEV Plus in batch mode.
- [TCAD Layout Reader on page 855](#) presents the TCAD layout reader of Sentaurus Process that provides a file-based interface between ICWBEV Plus and Sentaurus Process.

## Introducing ICWBEV Plus for TCAD Users

Before discussing the ICWBEV Plus–TCAD Sentaurus interface, it is important to have an understanding of ICWBEV Plus itself.

The general ICWBEV Plus training is a good starting point. Here, the focus is mainly on ICWBEV Plus operations that are most relevant to TCAD Sentaurus users.

For details, refer to the ICWBEV Plus documentation available from the **Help** menu. For all user documentation, choose **Help > Documentation**.

The first step consists of opening a layout file, which is typically in GDSII format.

---

## Opening GDSII Layout Files

To open a GDSII or an OASIS layout file:

1. On the command line, set the environment variable `ICWBEV_USER` to activate the ICWBEV Plus Sentaurus User Mode by typing:

```
setenv ICWBEV_USER SENTAURUS
```

2. Launch ICWBEV Plus by typing:

```
icwbev
```

3. Select the file to be opened by choosing **File > Open**.

4. In the Open File dialog box, browse to the file you want to load.

5. Click **Open**.

## User Interface of ICWBEV Plus

Figure 131 shows the user interface of ICWBEV Plus and illustrates the typical layout of work, panes, and toolbars. The panes can be moved and reconfigured as needed.

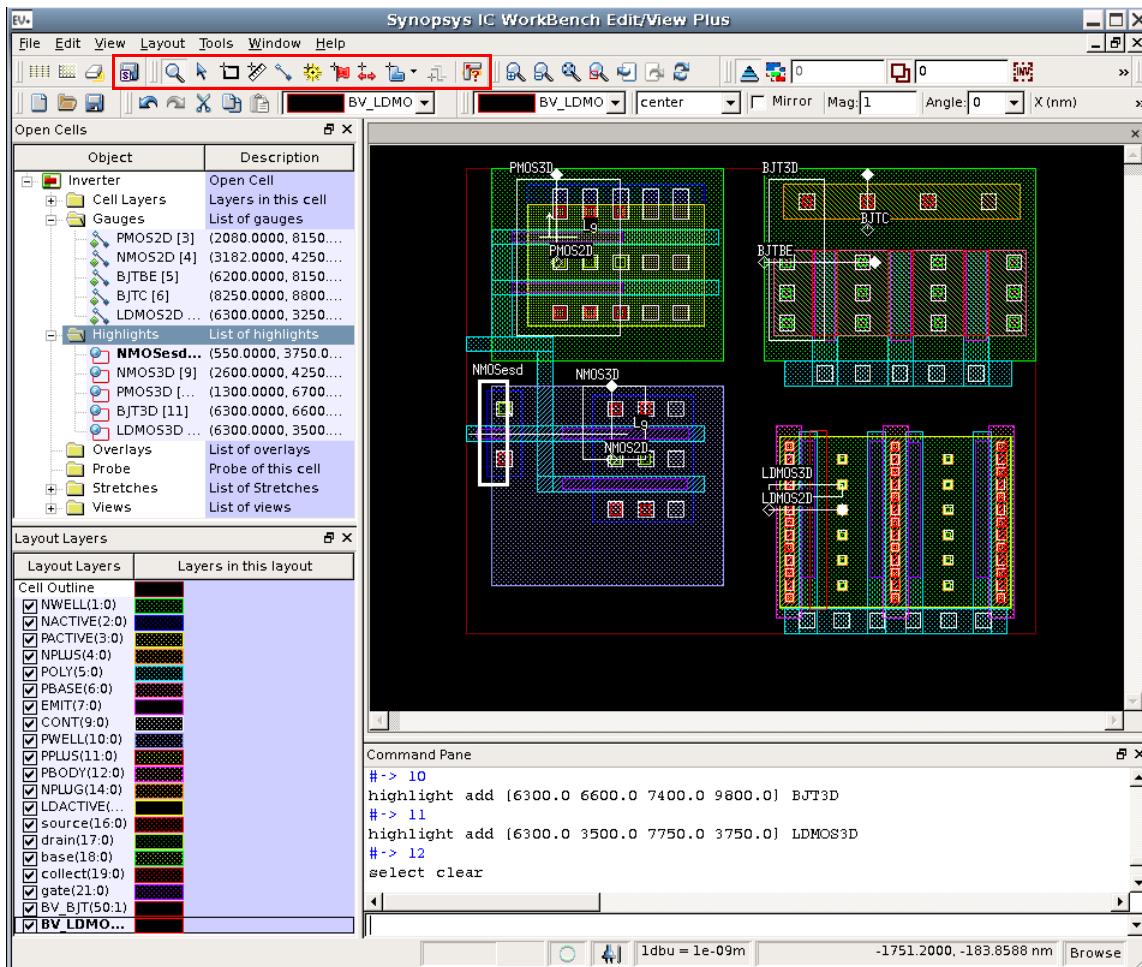


Figure 131 ICWBEV Plus main window with toolbar buttons specific to TCAD Sentaurus shown in red box at top

Figure 131 includes the following TCAD-relevant items in the GUI:

- The Open Cells pane contains details about layers and markups including the TCAD-relevant markups.
- The Layout Layers pane shows the list of layers.
- The Command Pane shows commands after GUI operations. Commands also can be entered directly in this pane.

## 13: ICWBEV Plus Interface for Layout-Driven Simulations

Introducing ICWBEV Plus for TCAD Users

**Table 95** describes the relevant buttons of the TCAD Sentaurus toolbar.

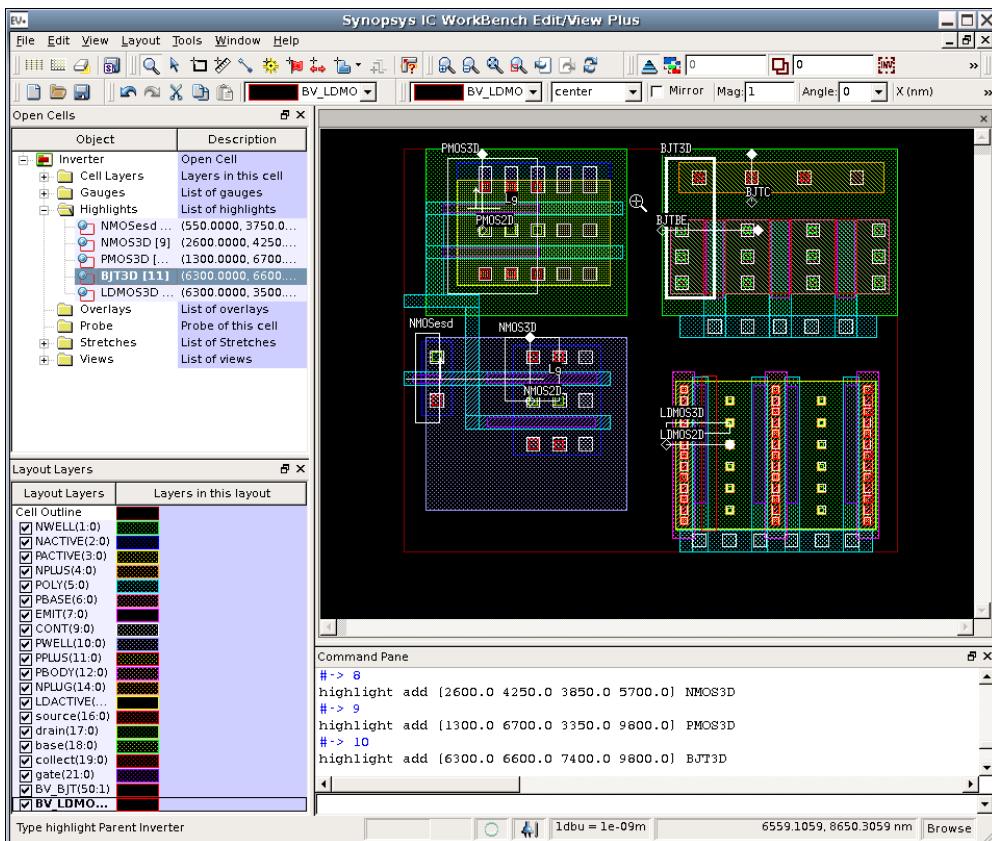
Table 95 TCAD Sentaurus-specific toolbar buttons

Button	Description	Button	Description
	Highlight (3D simulation domain)		Stretch utility
	Gauge (2D simulation domain)		Sentaurus Export for saving TCAD layout files or markup files
	Point (1D simulation domain)		

---

## Sentaurus Markups

Sentaurus markups are used to add the simulation domain in 1D, 2D, and 3D domains as needed. The Command Pane in [Figure 132](#) shows the commands after adding Sentaurus markups in the layout using GUI actions.



[Figure 132](#) Adding Sentaurus markups to a layout

To add a 3D simulation domain (highlight), a 2D simulation domain (gauge), or a 1D simulation domain (point), click the respective toolbar button and draw a rectangle, a line, or a point on the layout, respectively.

**NOTE** A 2D simulation domain (gauge) has a direction. The starting point is given as an open diamond, and the endpoint is given as a filled diamond. A gauge that runs parallel to an edge of a layer must have a finite orthogonal distance to that edge. If a gauge is collinear with the edges of a layer, this edge might not be included in the 2D mask.

The default naming convention is the following, where <n> is an automatically incremented number:

- For a highlight: SIM3D<n>
- For a gauge: SIM2D<n>
- For a point: SIM1D<n>

For 2D TCAD simulations, it can be useful to work with composite simulation domains, for example, when the different contacts in a device layout cannot be connected by a single straight line. In this case, it is not possible to perform a 2D device simulation after a 2D process step using a single 2D simulation domain. However, a 2D TCAD simulation using a composite 2D simulation domain is feasible. In this case, the various 2D cuts in the layout are joined to form a composite 2D simulation domain.

An example of a composite simulation domain is shown in [Figure 133](#), which shows a close-up of the layout of a bipolar transistor with two 2D TCAD simulation domains. The simulation domain labeled **BJTBE** cuts through two base-contact fingers and one emitter finger. The simulation domain labeled **BJTC** cuts through the collector contact.

**NOTE** The two simulation domains are orthogonal and not contiguous.

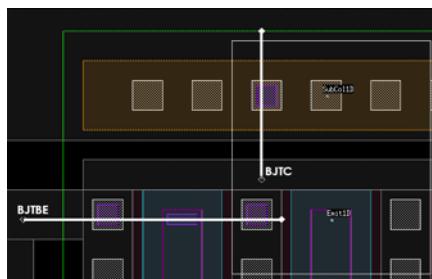


Figure 133 Layout of a bipolar transistor with two 2D simulation domains: BJTBE cuts through two base-contact fingers and one emitter finger, and BJTC cuts through the collector contact

## 13: ICWBEV Plus Interface for Layout-Driven Simulations

Introducing ICWBEV Plus for TCAD Users

Figure 134 shows the 2D TCAD simulation results obtained with a composite simulation domain consisting of both the BJTBE and BJTC domains. Using a composite simulation domain allows simulating a functional bipolar junction transistor (BJT) even for a 2D TCAD simulation.

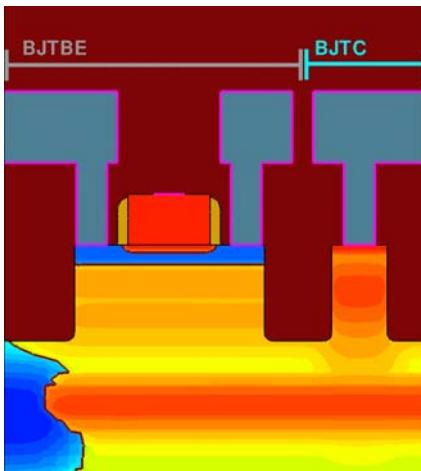


Figure 134 Two-dimensional TCAD simulation results using composite simulation domain consisting of the 2D domains BJTBE and BJTC

---

## Stretch Utility

The stretch utility provides a convenient way to parameterize a layout by inserting a uniformly stretched segment into the layout. For example, this feature can be used to generate a set of transistors that have different gate lengths but are otherwise identical.

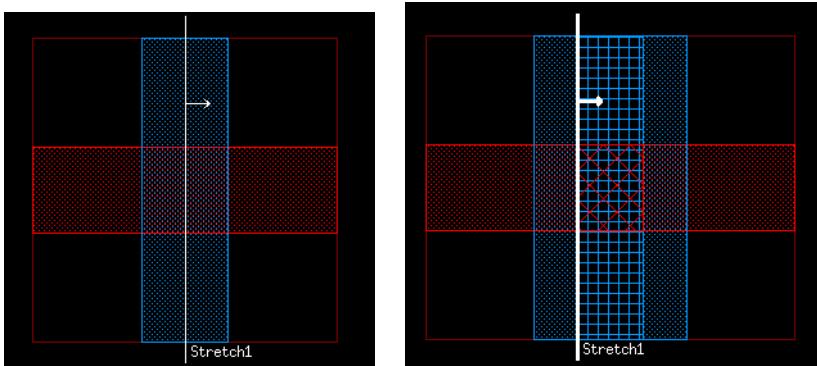


Figure 135 (*Left*) Snapshot of sample ICWBEV Plus layout with stretch utility line and (*right*) effective layout seen by Sentaurus Process when the layout is loaded with a positive stretch amount

A stretch line must be defined in ICWBEV Plus first. The stretch amount is set after loading the TCAD layout with the Sentaurus Process command:

```
icwb stretch name= "<stretch-name>" value= <stretch-amount>
```

This feature can be used for simple parameterization of layouts for quantities such as gate length (roll-off). [Figure 136](#) shows a close-up of the layout containing an NMOS transistor. In addition, two stretch lines are shown. The stretch line labeled NMOS\_W is used to vary gate width, and the one labeled NMOS\_L is used to vary the gate length in an NMOS.

To add a stretch line:

- Click the stretch utility toolbar button, and draw a line across the required region in the layout.

**NOTE** The stretch line must cross the entire simulation domain to which it should be applied. Stretch lines can be used for 2D and 3D simulation domains.



Figure 136 Adding stretch lines in a layout to vary gate width and gate length

[Figure 137 on page 842](#) shows the resulting changes in the NMOS gate width and gate length. The default naming scheme for a stretch line is `Stretch<n>`.

For example, to apply a stretch at runtime in Sentaurus Process, use a command such as:

```
icwb stretch name= "NMOS_W" value= @Stretch@
```

## 13: ICWBEV Plus Interface for Layout-Driven Simulations

Introducing ICWBEV Plus for TCAD Users

where NMOS\_W is the name of the stretch variable. Here, the amount of stretching is defined using the Sentaurus Workbench variable @Stretch@. A positive stretch value is used for expansion; a negative value leads to shrinkage.

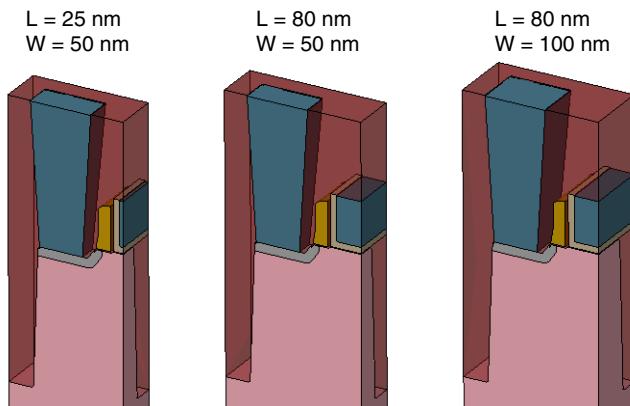


Figure 137 Effect of stretch utility on 3D NMOS structure showing variation in width and length

---

## Renaming Markups

Markups can be renamed and edited.

To rename markups:

1. Choose **View > Views > Open Cells**.
2. Expand the markup type, for example, **Highlights**.
3. Click the respective Sentaurus Process markup to edit the name.
4. Click the coordinates to edit the coordinate values.

[Figure 138 on page 843](#) shows the Open Cells pane, displaying the list of Sentaurus Process markups and their coordinates that can be edited as required.

Object	Description
Open Cell	Layers in this cell
Inverter	Open Cell
+ Cell Layers	Layers in this cell
+ Gauges	List of gauges
PMOS2D [3]	(2080.0000, 8150.0000)(2080.0000, 9900.0000) nm
NMOS2D [4]	(3182.0000, 4250.0000)(3182.0000, 5700.0000) nm
BJTBE [5]	(6200.0000, 8150.0000)(8400.0000, 8150.0000) nm
BJTC [6]	(8250.0000, 8800.0000)(8250.0000, 9900.0000) nm
LDMOS2D [7]	(6300.0000, 3250.0000)(7750.0000, 3250.0000) nm
+ Highlights	List of highlights
NMO5esd [8]	(550.0000, 3750.0000)(1100.0000, 5800.0000) nm
NMOS3D [9]	(2600.0000, 4250.0000)(3850.0000, 5700.0000) nm
PMOS3D [10]	(1300.0000, 6700.0000)(3350.0000, 9800.0000) nm
BJT3D [11]	(6300.0000, 6600.0000)(7400.0000, 9800.0000) nm
LDMOS3D [...]	(6300.0000, 3500.0000)(7750.0000, 3750.0000) nm
+ Overlays	List of overlays
+ Probe	Probe of this cell
+ Stretches	List of Stretches
Lg [1]	(350.0000, 4750.0000) (3500.0000, 4750.0000) nm
Lg [2]	(1750.0000, 8650.0000) (2500.0000, 8650.0000) nm
+ Views	List of views

Figure 138 Open Cells pane showing list of objects with descriptions

## Auxiliary Layers

Auxiliary layers are used, for example, to denote the position of electrical contacts in a layout. To add auxiliary layers, first a layer must be declared and attributes must be defined.

To add auxiliary layers, draw a polygon defining the region of the layer:

1. Open the layout for editing by choosing **Edit > Cell**.
2. Select the active layer.
3. Select the shape tool.
4. Draw a polygon.

## 13: ICWBEV Plus Interface for Layout-Driven Simulations

Introducing ICWBEV Plus for TCAD Users

Figure 139 illustrates how to define a layer and its attributes.

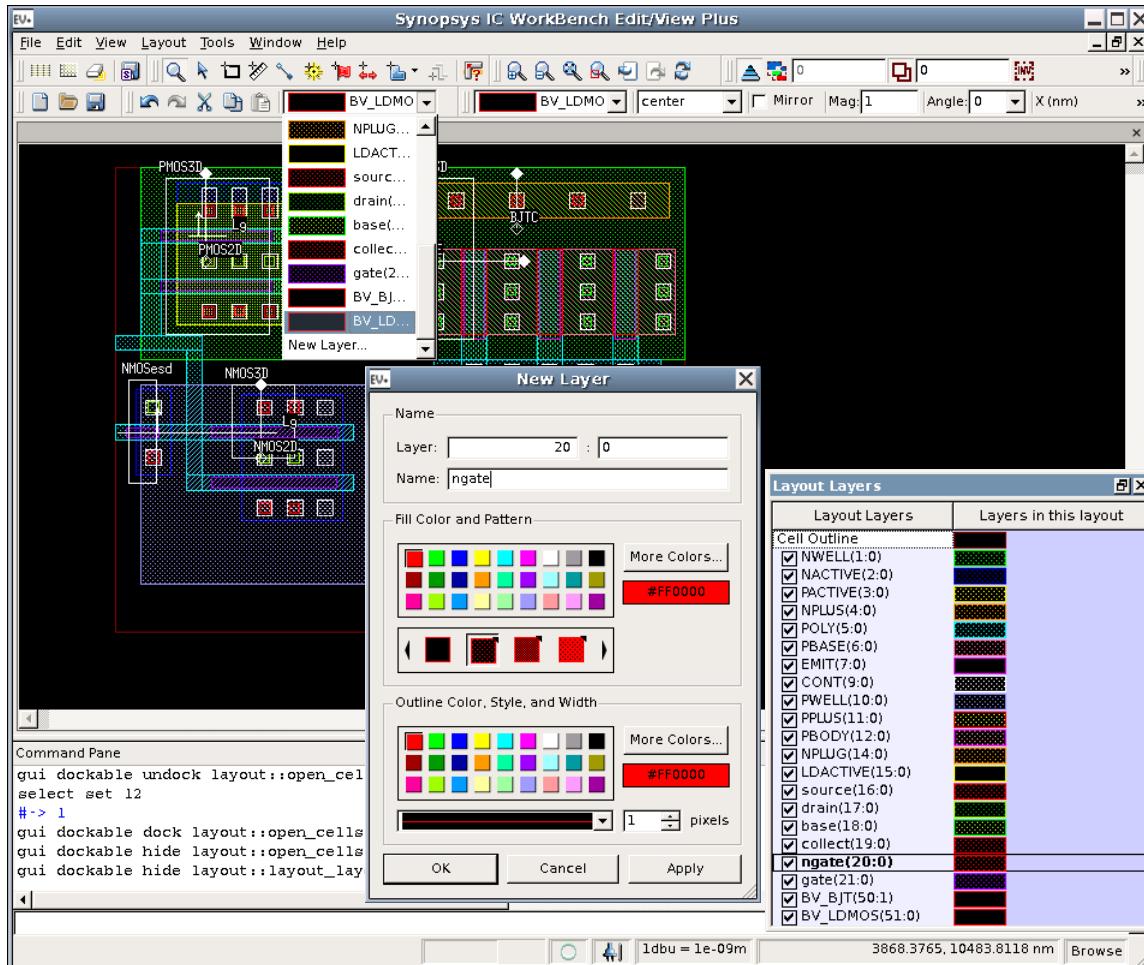


Figure 139 Defining a layer and its attributes: selecting New Layer, specifying attributes of layer, and Layout Layers panel showing new layer

---

## Text Labels

As an alternative to auxiliary layers, you can use text labels to denote the position of electrical contacts in a layout.

To add a text label:

1. Open the layout for editing by choosing **Edit > Cell**.
2. Select the active layer.
3. Select the text-adding tool by choosing **Tools > Create > Text**.

4. In the layout window, click at the location where you want to add the text label.
5. Type the name of the text label in the entry box.

---

## Editing Polygons

If required, polygons can be edited. You can edit polygons by either:

- Resizing a rectangle.
- Converting a rectangle to a polygon.

### Resizing a Rectangle

To resize a rectangle:

1. If not already open, open the layout for editing by choosing **Edit > Cell**.
2. Activate the selector tool.
3. Click the polygon edge to select it.
4. Move the edge as needed.

[Figure 140](#) shows a rectangle highlighted for editing.

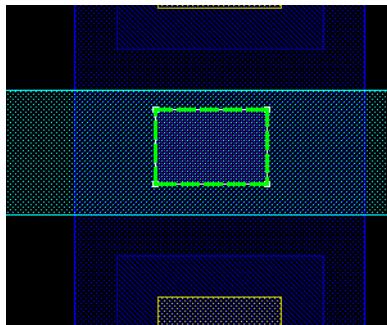


Figure 140 Moving the edge of a rectangle: select the rectangle and drag an edge

### Converting a Rectangle to a Polygon

To convert a rectangle to a polygon:

1. Click the polygon edge to select it.
2. Right-click and select **Split Edge**.
3. Move the edge as needed.

## 13: ICWBEV Plus Interface for Layout-Driven Simulations

Introducing ICWBEV Plus for TCAD Users

Figure 141 illustrates the procedure.

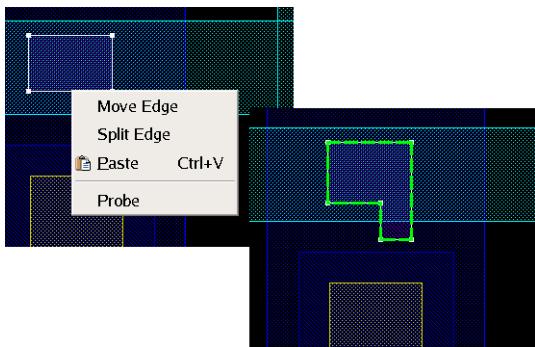


Figure 141 Converting a rectangle to a polygon

---

## Nonaxis-Aligned Simulation Domains

The ICWBEV Plus–TCAD Sentaurus interface supports nonaxis-aligned domains. To realize nonaxis-aligned simulation domains, the GDSII layout is rotated by a given angle, and the TCAD simulation domain is added as discussed in [Sentaurus Markups on page 838](#). [Figure 142 on page 847](#) shows the transformation of a GDSII layout and the transformation parameters.

To rotate a GDSII layout:

1. Choose **Layout > Transform**.
2. In the Transform dialog box, enter the values of the fields as required.
3. Click **OK**.

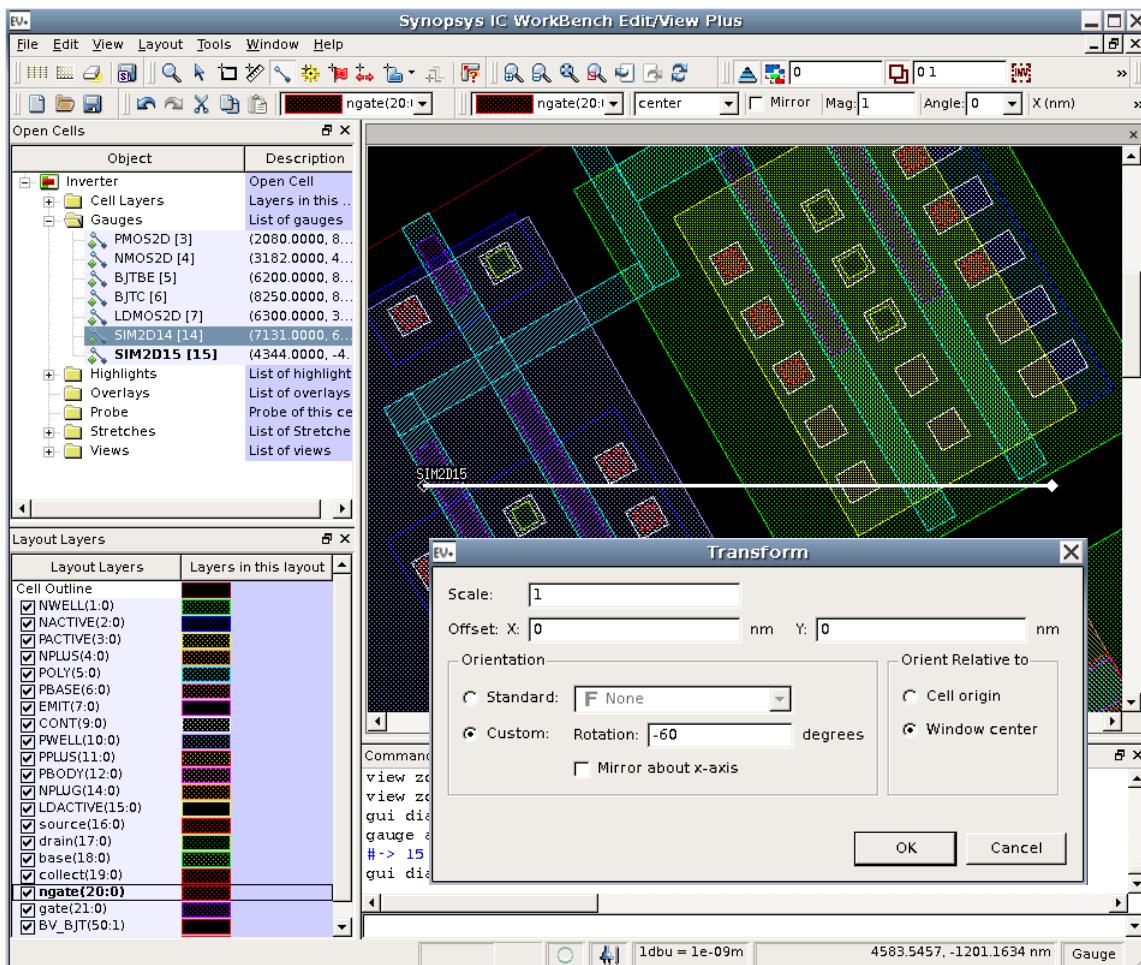


Figure 142 Rotation of layout with transformation parameters

## Sentaurus Markup Files and TCAD Layout Files

After adding Sentaurus Process markups in ICWBEV Plus, the markup information is saved in two different files:

- *Sentaurus markup file (\*.mfp.mac)*: This file format is based on the standard ICWBEV Plus macro language. It can be used to reload and re-edit Sentaurus Process markup. It also contains a reference to the original, potentially large, GDSII file.
- *TCAD layout file (\*.lyt.mac)*: This file format is used as an internal file format for the exchange of layout information between ICWBEV Plus and TCAD Sentaurus. It is based on the standard ICWBEV Plus macro language. This file is flat and does not contain a

## 13: ICWBEV Plus Interface for Layout-Driven Simulations

Sentaurus Markup Files and TCAD Layout Files

reference to the GDSII file. It is a small file because it contains only the parts of the layout needed for TCAD Sentaurus.

After performing the necessary operations on the layout file, save the resulting Sentaurus markup file.

---

## Saving the Sentaurus Markup File

To save a Sentaurus markup file:

1. Click the Sentaurus Export button (see [Table 95 on page 838](#)) or choose **Layout > Sentaurus Export**.
2. In the Sentaurus Export dialog box, select the **Markups** option (see [Figure 143 on page 849](#)).
3. If you have added auxiliary layers, which you do not want to store in the GDSII file, select the **Include new layers** option.

**NOTE** Including new layers in the markup file keeps the original GDSII file intact.

4. To open a specific layout file when reloading the markup file, select the **Open a layout file** option:
  - a) **Active layout:** Select this option when using a centrally located GDSII layout. This option is particularly useful when working with a very large full-chip layout.
  - b) **Layout:** Select this option when working with an edited or a local version of the GDSII layout. Specify the name of the layout.
5. Type the file name in the **Output file** field.

The recommended extension for saving the file is `_mfp.mac`, for example, `BiCMOS_mfp.mac`.

6. Click **OK**.

The corresponding script command is:

```
sentaurus export markups <name>_lyt.mac [-newLayers]
[-active | -reference <gdsfilename>]
```



Figure 143 Sentaurus Export dialog box, showing options for saving markup file

## Contents of Sentaurus Markup File

This section describes a typical markup file with a brief explanation. For a description of keywords, refer to the *IC WorkBench Edit/View Plus User Guide*.

Version information:

```
# Sentaurus markups information - Tue Jul 18 15:43:47 2017
# Version - M-2016.12 (513586)
```

Setting for treating self-intersection: By default, all layers are ORed. This convention is expected by all subsequent tools and, therefore, this setting should not be altered.

```
default winding 1
```

Pointer to layout file:

```
layout open [<path>]/BICMOSinverter.gds Inverter
```

Global transformations:

```
cell transform 1 0 0 0 0
```

Layer declarations and display settings:

```
layer configure 1:0 -name NWELL -fill #00ff00 -pattern fill12-a
-outline #00ff00 -lineStyle solid -lineWidth 1
```

## 13: ICWBEV Plus Interface for Layout-Driven Simulations

Sentaurus Markup Files and TCAD Layout Files

Open cell for editing (here, for adding new polygons):

```
cell edit_state 1
```

Auxiliary layers:

```
polygon -layer 20:0 {950 5150 950 5350 1150 5350 1150 5150}  
...
```

Simulation domains:

```
point add {8900 8100} Emit1D  
gauge add {2100 7900 2100 10000} PMOS  
highlight add {7900 7550 9900 9900} BJT3D  
...
```

Text labels:

```
cell object add text {layer 9:3 string "gate" coords {750 150}  
mag 0.3 anchor c angle 0 mirror 0}  
...
```

File end:

```
select clear  
catch {view default}
```

---

## Reloading the Markup File

To edit a markup file, you must reload it.

To reload a markup file:

1. Choose **File > Open**.

The Open File dialog box is displayed (see [Figure 144 on page 851](#)).

2. In the **Files of type** field, select **Flags Files (\*.mac)** or **Macro Files (\*.mac)**.
3. Select the file required.
4. Click **Open**.

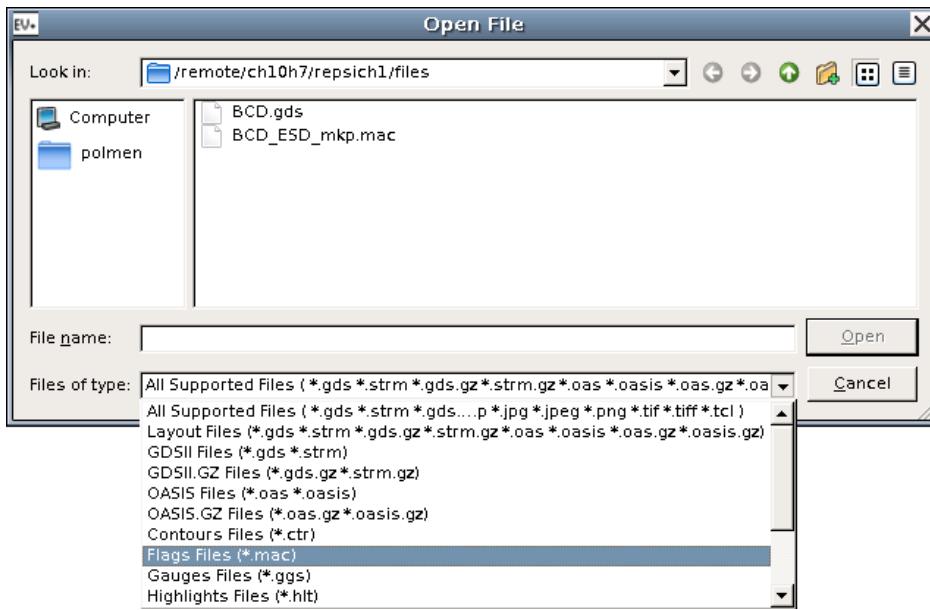


Figure 144 Open File dialog box for reloading markup file

## Saving the TCAD Layout File

To save the TCAD layout file:

1. Click the Sentaurus Export button (see [Table 95 on page 838](#)) or choose **Layout > Sentaurus Export**.
2. In the Sentaurus Export dialog box, select the **TCAD layout** option (see [Figure 145 on page 852](#)).
3. A layer in a layout can be defined by a large number of touching or overlapping polygons. To merge all these polygons into a smaller number of possibly more complex polygons, select the **Merge shapes** option.
4. For better viewing, layers are padded 10 units (nm). To change the padding value, edit the **Margin** field.
5. Type the file name in the **Output file** field.

The recommended extension for the TCAD layout file is `_lyt.mac`, for example, `BiCMOS_lyt.mac`.

6. Click **OK**.

The corresponding script command is:

```
sentaurus export layout <name>.lyt.mac [-merge | -noMerge] [-margin <number>]
```

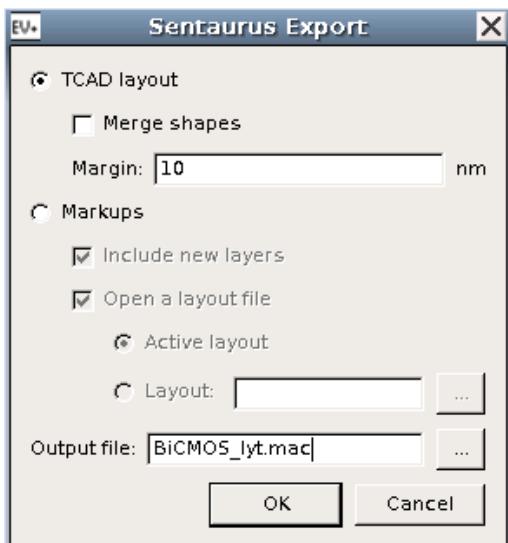


Figure 145 Sentaurus Export dialog box, showing options for saving TCAD layout file

---

## Contents of TCAD Layout File

This section describes the contents of the TCAD layout file and the differences between the contents of the Sentaurus markup file and TCAD layout file.

Version information: Same as [Contents of Sentaurus Markup File on page 849](#).

Setting for treating self-intersection: Same as [Contents of Sentaurus Markup File](#).

Pointer to layout file: Commented out.

Global transformations: Commented out.

Initialization of this self-contained layout:

```
layout new <cell name> -dbu 1e-09
```

Layer declarations and display settings: Same as [Contents of Sentaurus Markup File](#).

File end: same as [Contents of Sentaurus Markup File](#).

Simulation domains in a layout file are described below. Point, gauge, and highlight coordinates are mentioned first, and all polygons associated with the given simulation domains are listed:

- 1D simulation domains:

```
point add {8900 8100} Emit1D  
polygon -layer 1:0 {8890 8090 8910 8090 8910 8110 8890 8110}  
...
```

- 2D simulation domains:

```
gauge add {2100 7900 2100 10000} PMOS  
rectangle -layer 1:0 {2090 10010 2110 7890}  
...
```

- 3D simulation domains:

```
highlight add {7900 7550 9900 9900} BJT3D  
polygon -layer 1:0 {7890 7540 9910 7540 9910 9910 7890 9910}  
...
```

- Text labels:

```
cell object add text {layer 9:3 string "gate" coords {750 150}  
mag 0.3 anchor c angle 0 mirror 0}  
...
```

---

## Reloading the TCAD Layout File

For debugging purposes, reload the TCAD layout file.

To reload the file:

1. Choose **File > Open**.

The Open File dialog box is displayed (see [Figure 144 on page 851](#)).

2. In the **Files of type** field, select **Macro Files (\*.mac)**.

3. Select the required file.

4. Click **Open**.

**NOTE** Do not extract a TCAD layout from a reloaded TCAD layout. TCAD layout files should always be extracted from the Sentaurus markup file.

## 13: ICWBEV Plus Interface for Layout-Driven Simulations

Starting ICWBEV Plus in Batch Mode and Using Macros

---

# Starting ICWBEV Plus in Batch Mode and Using Macros

To extract the TCAD layout file in batch mode, add the following command to the end of the markup file:

```
sentaurus export layout <name>_lyt.mac [-merge | -noMerge] [-margin <number>]  
exit
```

To start ICWBEV Plus in batch mode, run the following command from the shell prompt:

```
> icwbev -nodisplay -run <name>_mfp.mac
```

---

## ICWBEV Plus Macros

ICWBEV Plus macros can be used to create simple layouts. An example of a macro is:

```
default winding 1  
layout new a -dbu 1e-09  
cell transform 1.0 0.0 0 0.0 0.0  
layer add 0:0  
layer configure 0:0 -name {} -fill #ff0000  
layer add 1:0  
layer configure 1:0 -name {} -fill #ff0000  
cell edit_state 1  
polygon -layer 0:0 {0 0 0 100 50 100 50 0}  
polygon -layer 1:0 {-25 25 75 25 75 75 -25 75}  
select clear  
catch {view default}
```

---

## Tcl-Based Macros for Layout Parameterization

The macro language of ICWBEV Plus is Tcl based. [Figure 146 on page 855](#) shows a rectangle that has been replicated four times. The following Tcl command performed the replication:

```
layout new a -dbu 1e-09  
layer configure 0:0 -name {}  
cell edit_state 1  
set SHIFTS [list 0 100 200 300 400]  
foreach SHIFT $SHIFTS {  
    eval rectangle -layer 0:0 { $SHIFT 0 [expr 50+$SHIFT] 50 }  
}
```

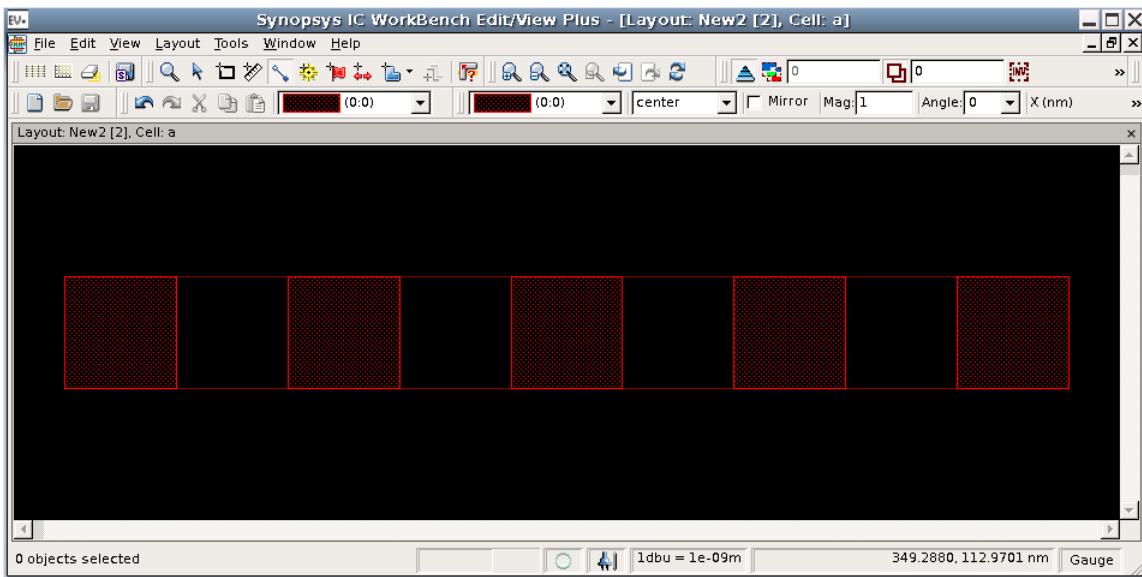


Figure 146 Shift operation using macros

---

## TCAD Layout Reader

The TCAD layout reader of Sentaurus Process provides a file-based interface between ICWBEV Plus and Sentaurus Process. Some of its key features include:

- Loading the TCAD layout (optional rescaling)
- Layout query functions
- Selecting a simulation domain
- Applying stretches
- Creating masks
- Mask-driven meshing
- Mask-driven contact assignment

The following sections discuss these features in detail.

## Loading the TCAD Layout

To load a TCAD layout in Sentaurus Process, use the command:

```
icwb filename=<c> [scale=<n>]
```

Coordinates found in the TCAD layout file are multiplied by the value of the optional argument scale as the file is read.

For example, to load the TCAD layout file `BiCMOS_lyt.mac` and to apply a rescaling factor of 1/1000 to convert the ICWBEV Plus default unit of nanometer to the Sentaurus Process default unit of micrometer, use:

```
icwb filename= "BiCMOS_lyt.mac" scale= 1e-3
```

---

## Finding Simulation Domains

To generate a list of the simulation domains, use:

```
icwb list domains
```

For example:

```
set Domains [icwb list domains]
-> icwb: Domains -> Emit1D NBODY NMOS BJT3D PMOS3D
```

---

## Finding Layer Names and Layer IDs

Each layer in the TCAD layout file has a unique ID of the form `<integer>:<integer>`, for example `3:0`. A layer also can have an optional explicit layer name such as `NWELL`. If no explicit layer name has been set in ICWBEV Plus, the TCAD layout reader uses the layer ID as the default layer name. The TCAD layout reader refers to layers always by the layer name.

To find the layer names, use:

```
icwb list layerNames
```

For example:

```
set LNames [icwb list layerNames]
-> icwb: LNames -> NWELL NPDIFF POLY EMIT METAL CONT ndrain ngate nsource base
emitter collect
```

To find the layer IDs, use:

```
icwb list layerIDs
```

For example:

```
set LIDs [icwb list layerIDs]
-> icwb: LIDs -> 1:0 2:0 3:0 4:0 5:0 6:0 7:0 8:0
```

---

## Selecting the Simulation Domain

To select a single or a composite simulation domain, use one of the following commands:

```
icwb domain=<c> | <list-of-2d-domain-names>
icwb domain= { <domain_name1> <domain_name2> ...<domain_namen> }
```

For example, to select a single simulation domain (which can be 1D, 2D, or 3D), use:

```
icwb domain= {PMOS}
```

To define a composite simulation in two dimensions, use:

```
icwb domain= { NBODY NMOS PMOS BJTBE BJTC }
```

---

## Loading a GDSII Layout

To load a GDSII layout directly in Sentaurus Process, use the command:

```
icwb gds.file=<c> cell=<c> layer.names= {<list>} layer.numbers= {<list>}
sim2d | sim3d= {<n>} [domain.name=<c>] [scale= <n>]
[stretches= {<c>= {<n>}}]
```

For example:

```
icwb gds.file= BCD.gds cell= Inverter \
layer.numbers= "1:0 2:0 3:0 4:0 5:0 6:0 7:0 8:0" \
layer.names= "NWELL NACTIVE PACTIVE NPLUS POLY PBASE EMIT CONT" \
sim3d = "6300 3500 7750 3750" \
stretches= {lgate= {7025 3400 7025 3850}} scale= 1e-3
```

The `domain.name` argument defines the name of the simulation domain. If no name is specified, `SIM3D` is used for a 3D domain, and `SIM2D` is used for a 2D domain.

The domain will be set to be the current domain automatically, so you do not need to call `icwb domain=<c>` before using other `icwb` commands.

**NOTE** The simulation domain and the stretches are defined using layout coordinates. This option does not require access to ICWBEV Plus. Two-dimensional composite simulation domains are supported using a variation of the `icwb` command (see [icwb.composite on page 992](#)).

---

## Finding Domain Dimensions

To find the domain dimensions, use:

```
icwb dimension
```

This command returns 3 for 3D simulation domains (highlight), 2 for 2D simulation domains (gauge), and 1 for 1D simulation domains (point).

For example:

```
set DIM [icwb dimension]
-> icwb: dimension -> 3
```

---

## Finding Bounding Box of Domain

To find the coordinates of the bounding box of the simulation domain in the global layout coordinates, use:

```
icwb bbox (xmin | xmax | ymin | ymax)
```

For example:

```
set LXmin [icwb bbox xmin] ; set LXmax [icwb bbox xmax]
set LYmin [icwb bbox ymin] ; set LYmax [icwb bbox ymax]
-> icwb: Layout Bounding Box -> 7.9 9.9 7.55 9.9
```

To find the coordinates of the bounding box that automatically recenters the simulation domain to start at the origin, use:

```
icwb bbox (left | right | back | front)
```

For example:

```
set Ymin [icwb bbox left] ; set Ymax [icwb bbox right]
set Zmin [icwb bbox back] ; set Zmax [icwb bbox front]
-> icwb: Centered Bounding Box -> 0 2.35 0 2
```

**NOTE** Sentaurus Process works with the centered coordinates. The coordinates in Sentaurus Process correspond to `left`, `right`, `front`, and `back`. Whereas, GDS layout coordinates correspond to `xmin`, `ymin`, `xmax`, and `ymax`. In other words,  $(0, 0)$  corresponds to  $(7.9 \ 9.9)$  on the layout. The option `!recenter` can be given with the `gds .file` or `filename` argument to switch off recentering, which is supported in 3D simulations.

---

## Interface With line Commands

After storing the bounding box of the simulation domain in the Tcl variables such as `Ymin`, `Ymax`, `Zmin`, and `Zmax`, these variables can be used in `line` commands to define the initial substrate and mesh in Sentaurus Process. For example:

```
if { $DIM == 3 } {
    line y location= $Ymin spacing=100.0 tag=left
    line y location= $Ymax spacing=100.0 tag=right
    line z location= $Zmin spacing=100.0 tag=back
    line z location= $Zmax spacing=100.0 tag=front
    set Ydim "ylo=left yhi=right"
    set Zdim "zlo=back zhi=front"
} elseif { $DIM == 2 } {
    line y location= $Ymin spacing=100.0 tag=left
    line y location= $Ymax spacing=100.0 tag=right
    set Ydim "ylo=left yhi=right"
    set Zdim ""
} else {
    line y location=-0.5 spacing=100.0 tag=left
    line y location= 0.5 spacing=100.0 tag=right
    set Ydim "ylo=left yhi=right"
    set Zdim ""
}
eval region silicon xlo=top xhi=bottom $Ydim $Zdim
```

---

## Creating Masks

To create a mask from a layer, use the command:

```
icwb.create.mask
layer.name= <c> | <list>
[name= <string>] [polarity= positive | negative]
[save.to.tdr= 0 | 1]
[shift= {<dy> <dz>}]
[stretchypos= {<yo> <dy>}] [stretchyneg= {<yo> <dy>}]
```

## 13: ICWBEV Plus Interface for Layout-Driven Simulations

### TCAD Layout Reader

```
[stretchzpos= {<zo> <dz>}] [stretchzneg= {<zo> <dz>}]
[reflecty= <yo>] [reflectz= <zo>]
```

Masks can be created in the following ways:

- Mask name defaults to the layer name:

```
icwb.create.mask layer.name= POLY
```

- Give an explicit name to the mask. For example, to distinguish between the positive mask and negative counterparts:

```
icwb.create.mask layer.name= NWELL name= NWELL polarity= positive
icwb.create.mask layer.name= NWELL name= NOTNWELL polarity= negative
```

Several layers can be *OR*ed to create a single mask. The following command illustrates the OR procedure:

```
icwb.create.mask layer.name= "NPDIFF PPDIFF NPLUG PBASE" name= STI info= 1
```

The `info` argument directs more detailed information about the mask creation process to the log file.

To automatically create mask layers with both polarities, use the command:

```
icwb.create.all.masks
```

The resulting mask names are `<layername>_p` for the positive version and `<layername>_n` for the negative version.

The optional arguments `shift`, `stretchypos`, `stretchyneg`, `stretchzpos`, and `stretchzneg`, `reflecty`, and `reflectz` allow you to modify individual layers during the mask generation with `icwb.create.mask`. For example, to generate a mask that corresponds to layer `1:0` shifted by  $0.25 \mu\text{m}$  along the y-direction and by  $-0.1 \mu\text{m}$  along the z-direction, use:

```
icwb.create.mask layer.name= 1:0 shift= {0.25 -0.1}
```

For 2D simulation domains, the z-shift can be omitted.

The arguments starting with the word `stretch` allow you to stretch individual layers in a manner similar to the `icwb stretch` command. (The latter, however, is applied to all layers and takes the location of the stretch from the TCAD layout file.) The remaining part of the argument determines whether the stretch is applied along the y- or z-direction, and whether the layer is stretched to the positive or negative side of the stretch position. For example, to move the vertices of layer `1:0`, which have a y-coordinate less than  $1.2$  by  $-0.25 \mu\text{m}$ , use:

```
icwb.create.mask layer.name= 1:0 stretchyneg= {1.2 -0.25}
```

This command operates on layer vertex coordinates and does not check if the resulting polygon is valid. When using these commands to shrink layers, you must ensure that the resulting polygons are still well defined, for example, not self intersecting.

More than one `shift`, `stretch*`, and `reflect*` argument can be used in the `icwb.create.mask` command. As these operations may not commute, you must note the order in which these operations are applied if more than one is used. First, `shift` is applied, and then `stretchypos`, `stretchyneg`, `stretchzpos`, `stretchzneg`, `reflecty`, and finally `reflectz` are applied.

**NOTE** This order is hard coded and not influenced by the order the arguments appear on the command line.

**NOTE** If you have a large layout with masks containing many polygons, it can take some time until the Tcl function `icwb.create.all.masks` parses and creates the masks. In this situation, you can use the command `icwb create.all.masks` to create all the masks (see [icwb on page 988](#)). This command works like the Tcl version but creates the masks much faster.

By default, all masks are saved into a TDR file and can be reused after reloading the TDR file in a different input file. Certain GDSII files can, however, contain layers with a very large number of points. Saving masks created from such GDSII layers in a TDR file is usually undesirable and is automatically suppressed. The default of the cut-off limit is 200 points per layer. If needed, you can increase this limit with:

```
pdbSet GDS Max.Points <n>
```

In addition, you can suppress the saving *any* mask created from GDSII layers by setting:

```
pdbSetBoolean GDS Save.To.TDR 0
```

To overwrite the default saving behavior for an individual mask, use the `save.to.tdr` argument, for example:

```
icwb.create.all.masks save.to.tdr= 0 | 1
icwb.create.mask layer.name= L012 name= L012_n polarity= negative \
    save.to.tdr= 0 | 1
```

**NOTE** If you have a large layout with masks containing many polygons, it can take some time until the `icwb.create.all.masks` Tcl function parses and creates the masks. In this situation, you can use the command `icwb create.all.masks` to create all the masks (see [icwb on page 988](#)). This command works like the Tcl version but creates the masks much faster. Masks created with the `icwb create.all.masks` command are not saved to the TDR file.

## Mask-Driven Meshing

To create a refinement box that is tied to a mask, use:

```
refinebox
[(mask=<c> extrusion.min=<n> extrusion.max=<n>) [extend=<n>]
 ([mask.corner.mns=<n>] [mask.corner.ngr=<n>]
 [mask.corner.refine.extent=<n>] |
 [mask.edge.mns=<n>] [mask.edge.ngr=<n>] [mask.edge.refine.extent=<n>]) ]
[<other_arguments>]
```

Mask-driven meshing can be particularly useful when meshing in critical regions, such as the channel and emitter areas of BiCMOS devices. The following example illustrates the use of the POLY mask for meshing placement:

```
refinebox name= UnderPoly mask= POLY extend= 0.1 \
extrusion.min= -1.51 extrusion.max= -1.35 \
xrefine= 0.02 yrefine= 0.02

refinebox name= SiOxPo mask= POLY extend= 0.1 \
extrusion.min= -1.51 extrusion.max= -1.35 min.normal.size= 0.005 \
interface.mat.pairs= {Silicon Oxide Silicon Polysilicon}
```

The `extend` argument provides the option to mesh in areas wider than the mask.

[Figure 147](#) and [Figure 148 on page 863](#) demonstrate the use of the `extend` argument in the emitter region of a BJT and the channel region of an NMOS, respectively.

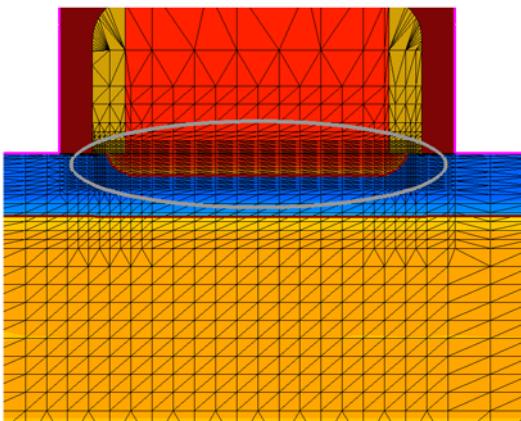


Figure 147 Meshing in emitter region of BJT; the `extend` parameter is set to 0.1  $\mu\text{m}$

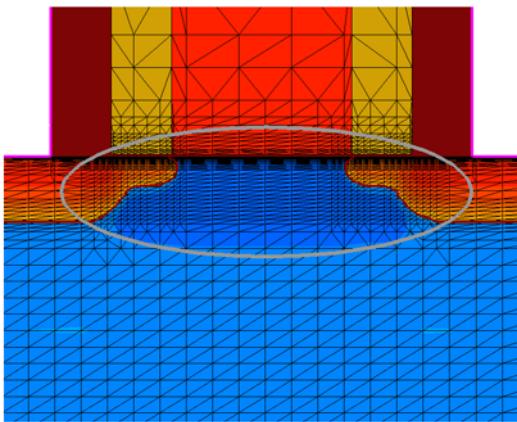


Figure 148 Meshing in channel region of NMOS; the extend parameter is set to 0.1  $\mu\text{m}$

## Layout-Driven Contact Assignment

The `icwb.contact.mask` command creates contacts for subsequent device simulations that are tied to a layer or a text label in the TCAD layout file. The command serves as an interface between the TCAD layout and the Sentaurus Process `contact` command by automatically obtaining the lateral placement of the contact from the specified layout layer or text label, taking the vertical placement from the argument list and passing all other options directly to the `contact` command. The syntax of the command is:

```
icwb.contact.mask
  (label.name=<c> [distance=<n>] | layer.name=<c>
   (box <material> [adjacent.material=<c>] [boxheight=<n>] [xhi=<n>] [xlo=<n>]
    |
    point <material> [replace] [x=<n>])
  [name=<c>] [<other_arguments>]
```

The `icwb.contact.mask` command supports both box-type and point-type contacts:

- A *box-type* contact consists of elements at the surface of one region or material inside the box. The lateral extent of the box is determined automatically from the layer segment (two dimensions) or the layer polygons (three dimensions), while the vertical extent is taken from the `xlo` and `xhi` arguments of the `contact` command. If the `xlo` argument is not explicitly given, the vertical extent is determined automatically, based on the topmost interface with the material mentioned in the command call. The vertical extent of the box is controlled by `boxheight`. If a text label name is given, the layer associated with that text label is used.
- A *point-type* contact contains all the boundary elements of one region. The lateral position of the point is determined automatically as a point inside the layer segment (two dimensions) or the polygon (three dimensions), while the vertical position is taken from the

## 13: ICWBEV Plus Interface for Layout-Driven Simulations

### TCAD Layout Reader

`x` argument of the `contact` command. If the `x` argument is not explicitly given, the vertical position is determined automatically, based on the interfaces with the material given in the command call. If a text label name is given, the anchor point of the text label is used.

Often, there is no layer or text label in the layout provided by designers that can be used readily for the creation of contacts. In this case, add auxiliary layers or text labels in ICWBEV Plus to be used as markups for device contacts.

The following example demonstrates the assignment of gate and drain contacts using layout-driven contact assignment:

```
icwb.contact.mask layer.name= ndrain name= drain point aluminum \
replace x= -2.0

icwb.contact.mask layer.name= ngate name= gate box polysilicon \
adjacent.material= oxide xlo= -2.05 xhi= -1.95

icwb.contact.mask label.name= "drain" point Aluminum replace
```

Any other commands not explicitly handled by the `icwb.contact.mask` command are passed to the `contact` command. The argument `name` is optional. If no `name` is given, the `label.name` or the `layer.name` is used as the contact name, depending on whichever has been specified.

[Figure 149 on page 865](#) shows a layout on which auxiliary layers have been added for layout-driven contact assignment. [Figure 150 on page 865](#) shows the 2D boundary after the process simulation with Sentaurus Process depicting the gate, drain, and source contacts.

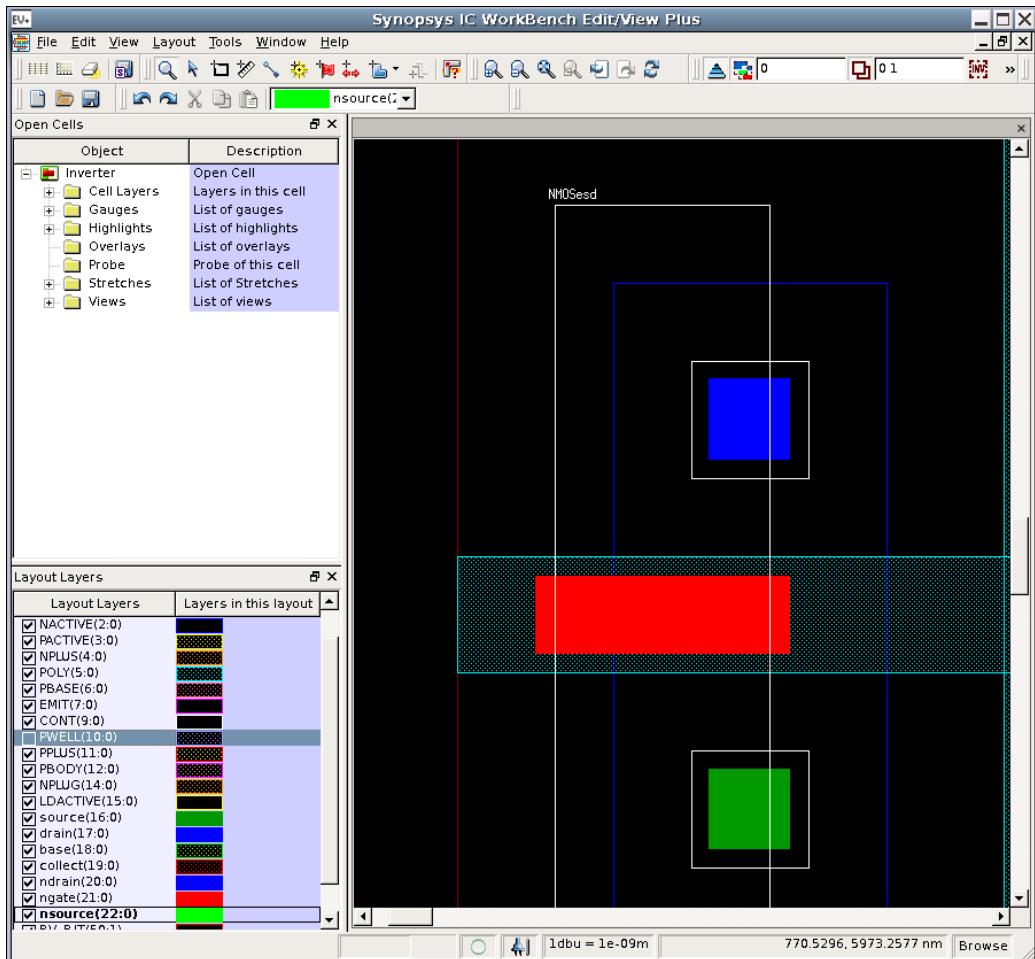


Figure 149 Auxiliary layers added for gate, source, and drain contacts are represented by rectangles of solid color in the layout

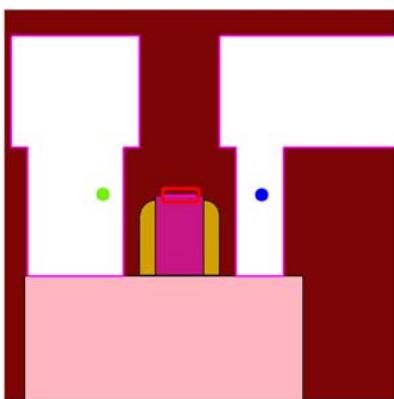


Figure 150 Final boundary after TCAD simulation showing gate (red), drain (blue), and source (green)

---

## Aligning Wafer and Simulation Domain

To correctly support tilted process steps for 2D and 3D simulation domains, the alignment between the wafer and the simulation domain must be declared using the `slice.angle` argument of the `init` command.

The TCAD layout reader command `icwb slice.angle.offset` returns the relative angle of the active simulation domain so that the slice angle can be adjusted as needed.

[Table 96](#) lists the returned `slice.angle` offset values for:

- A 3D simulation domain (`SIM3D1`).
- A 2D domain along the layout x-axis extending from left to right (`SIM2DXLR`) and from right to left (`SIM2DXRL`), and along the layout y-axis from top to bottom (`SIM2DYTD`) and from bottom to top (`SIM2DYDT`).

Table 96 Values of `slice.angle` offset for different domains

Domain	Offset value returned
<code>SIM3D1</code>	90
<code>SIM2DXLR</code>	0
<code>SIM2DXRL</code>	180
<code>SIM2DYDT</code>	90
<code>SIM2DYTD</code>	-90

The following commands realize a tilted process:

```
set SliceAngle -90
set SliceOffset [icwb slice.angle.offset]
init silicon field= Boron concentration= 1e13 \
    slice.angle= [expr $SliceAngle+$SliceOffset]
implant phosphorus dose= 4e12<cm-2> energy= 100<keV> tilt= 30 rotation= 0
```

[Figure 151 on page 867](#) shows a sample layout with a 3D simulation domain and the four 2D simulation domains previously discussed. [Figure 152 on page 867](#) and [Figure 153 on page 868](#) show the dopant profiles after the tilted implantations for the different simulation domains.

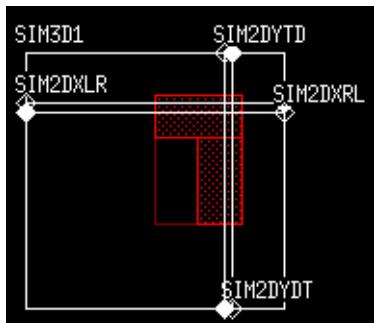


Figure 151 Structure layout where implantation is performed at highlighted L-shaped red region

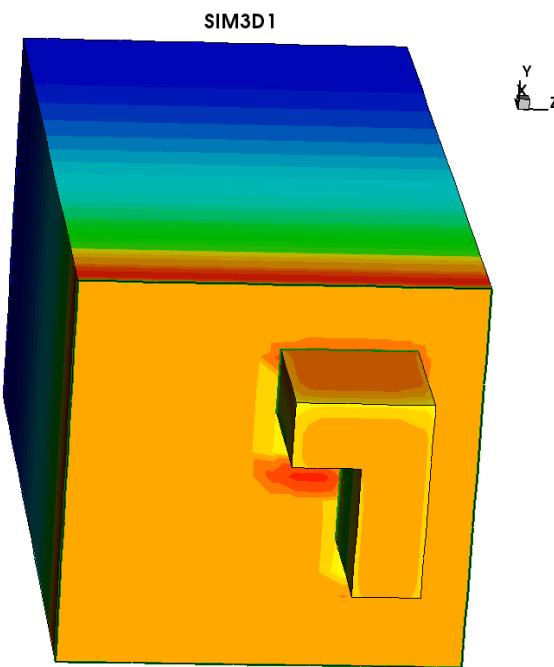


Figure 152 Three-dimensional implanted profile

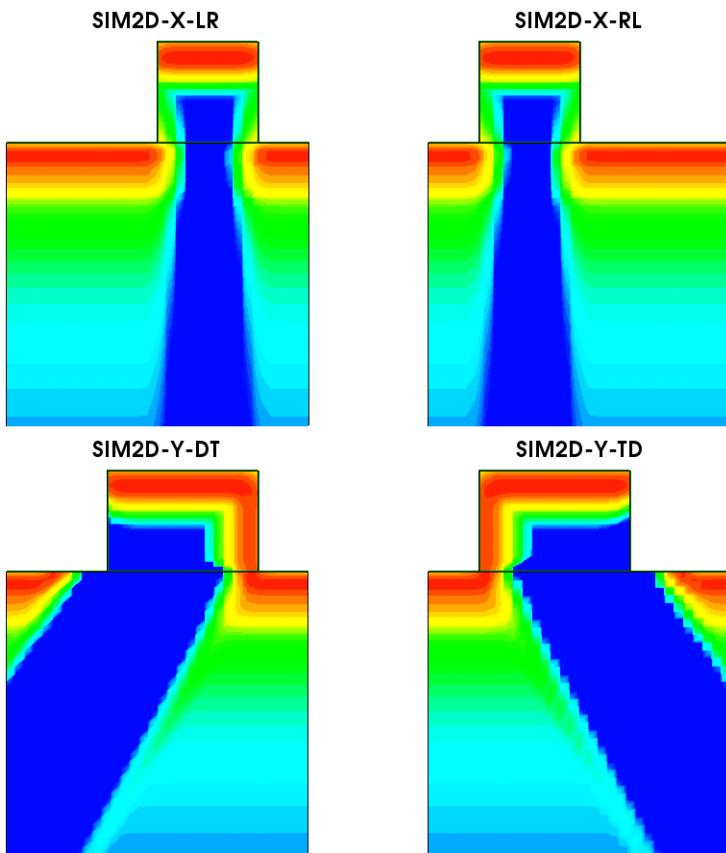


Figure 153 Two-dimensional implanted profile for selected slice angles as mentioned in [Table 96 on page 866](#)

---

## Additional Query Functions

The TCAD layout reader of Sentaurus Process provides additional layout query functions. For example, the following command returns a list of segments in the given layer for a 2D simulation domain:

```
set Segments [icwb list.segments layer.name= "<layer-name>"]
```

For a 3D simulation domain, the following command returns a list containing the bounding boxes for all polygons in the given layer (this command also can be used for 2D):

```
set PolyBBoxes [icwb list polygon.bounding.boxes layer.name= "<layer-name>"]
```

For a 3D simulation domain, the following command returns a list containing a tessellated representation of polygons in the given layer (this command also can be used for 2D):

```
set PolyTessel [icwb list polygon.tessellations layer.name= "<layer-name>"]
```

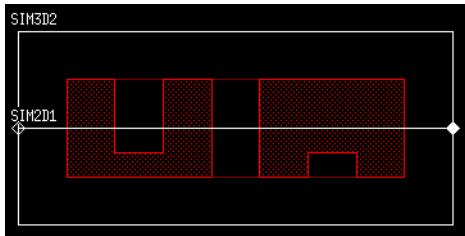


Figure 154 Sample layout containing two polygons

For example, [Figure 154](#) shows a simple layout containing two polygons in layer 0:0. The following commands:

- Load the TCAD layout file (here, called `ORG_lyt.mac`).
- Select the 2D simulation domain `SIM2D1`.
- Query the segment, the bounding boxes, and the tessellations:

```
icwb filename= "ORG_lyt.mac"
icwb domain= "SIM2D1"

set Segments [icwb list.segments layer.name= "0:0"]
LogFile "Segments $Segments"
# -> Segments 100 200 300 400 500 800

set BBoxes [icwb list polygon.bounding.boxes layer.name= "0:0"]
LogFile "BBoxes: $BBoxes"
# -> BBoxes: {100 0 200 0} {300 0 400 0} {500 0 800 0}

set Tessellations [icwb list polygon.tessellations layer.name= "0:0"]
LogFile "Tessellations: $Tessellations"
# -> Tessellations: {100 0 200 0} {300 0 400 0} {500 0 800 0}
```

**NOTE** The bounding box and tessellation queries are supported for 2D, and they return flat rectangles. The returned y-values are the same as for the segment query; however, zeros are padded for the z-direction.

When loading the 3D simulation domain `SIM3D2`, the set of rectangles returned by the `polygon.bounding.boxes` query and the `polygon.tessellations` query are different:

```
icwb filename= "ORG_lyt.mac"
icwb domain= "SIM3D2"

set BBoxes [icwb list polygon.bounding.boxes layer.name= "0:0"]
LogFile "BBoxes: $BBoxes"
# -> BBoxes: {100 100 300 400} {100 500 300 800}
```

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### TCAD Layout Reader

```
set Tessellations [icwb list polygon.tessellations layer.name= "0:0"]
LogFile "Tessellations: $Tessellations"
# -> Tessellations: {100 100 150 200} {100 200 150 300} {100 300 150 400}
# {100 500 150 600} {100 700 150 800} {150 100 300 200} {150 300 300 400}
# {150 500 300 600} {150 600 300 700} {150 700 300 800}
```

The `polygon.bounding.boxes` query returns the bounding box rectangle for each polygon in the layer, while the `polygon.tessellations` query breaks each polygon into a set of rectangles and then returns these rectangles. The set of rectangles covers the same area as the original polygon, while the bounding box rectangles may cover a larger area.

[Figure 155](#) shows the rectangles returned by the two query functions as an ‘effective/equivalent’ layout for better comparison with the original layout shown in [Figure 154 on page 869](#).

**NOTE** The tessellation procedure supports only polygons with axis-aligned edges.

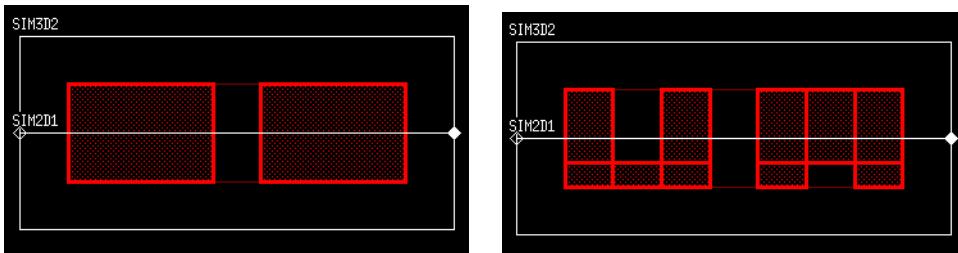


Figure 155 Set of rectangles returned by (*left*) `polygon.bounding.boxes` query and (*right*) `polygon.tessellations` query for polygons shown in [Figure 154](#)

# CHAPTER 14 Extracting Results

---

*This chapter presents strategies for analyzing simulation results.*

---

## Overview

This chapter covers basic tasks such as obtaining a list of materials currently in the structure, and obtaining 1D dopant profiles from 2D or 3D structures to more complex ones, such as looping through all materials and extracting Pearson parameters for each material. The following commands perform these tasks: `interface`, `interpolate`, `layers`, `mater`, `print.1d`, `select`, `slice`, `FitArrhenius`, `FitLine`, `FitPearson`, and `FitPearsonFloor`.

All these commands are built-in procedures designed to work with the tool command language (Tcl). These commands allow you to take full advantage of the programmability of the Sentaurus Process input language and provide a powerful framework for performing complex customized tasks.

These commands return or accept a Tcl list to perform their respective functions. The Tcl list can be viewed and processed by the user, passed to another function, written to a file, or read from a file. For example, the `slice` command returns a Tcl list of *xy* pairs where the *x* value gives the depth [ $\mu\text{m}$ ] and the *y* value gives the value chosen with the `select` command. This list can be viewed with the Tcl `puts` command, written to a file with the Tcl `open` and `puts` commands, or processed with another command such as fitting a Pearson function to the profile with the `FitPearson` command.

An understanding of basic Tcl commands and Tcl lists is helpful to utilize fully the flexibility of these commands. For convenience, some basic aspects of Tcl are described to enable you to work efficiently with these commands, and examples of basic results analysis are provided.

---

## Saving Data Fields

Sentaurus Process automatically saves all solutions, active dopant concentrations, total dopant concentrations, electrostatic potential, net active concentrations, point-defect concentrations, and total point-defect concentrations along with mechanical stress results in a TDR file. The total and active concentrations of dopants and the total concentration of defects are created only after a diffusion step. Therefore, if there is no diffusion, some of these fields may not be in the

## 14: Extracting Results

### Selecting Fields for Viewing or Analysis

TDR file. You can control the fields that will be saved in the TDR file using the `SetTDRList` command (see [SetTDRList on page 1187](#)).

Since the active and total dopant concentrations are defined as terms in Sentaurus Process, they are converted automatically to data fields with the same name when saved to TDR files. Because the conversion is handled internally, the data fields are not kept in the memory.

You can create new data fields and store them in a TDR file. The following example divides the active boron concentration by the total boron concentration, and saves the results in a data field called `BActiveRatio`:

```
sel z= "BActive/BTotal" name= BActiveRatio store
```

The parameter `store` ensures that the newly created field will be saved in a TDR file. To see whether a field will be saved in a TDR file, the `select` command with the option `permanent` can be used (see [select on page 1168](#)). The following example returns 1 if the field will be saved in a TDR file (otherwise, it returns 0):

```
sel name= BActiveRatio permanent
```

---

## Selecting Fields for Viewing or Analysis

Most analytic tasks begin with the `select` command, which is used to select a data field to be viewed or operated on (see [select on page 1168](#)). A data field in Sentaurus Process is a quantity that varies over the simulation domain, such as dopant concentration or electrostatic potential distribution. The value of the data field is defined with an Alagator expression and is set with the `z` parameter of the `select` command.

The expression can be simply the name of a solution variable (such as `Boron`, `H2O`, or `Stress_x`) or it can be a complex expression depending on what is required. If the expression is the simple name of an existing data field, the `select` command selects this data field.

If it is more complex expression, the `select` command creates a corresponding data field and then selects it, for example:

```
select z= BTotals          ;# Select the total boron concentration  
                      ;# term  
select z= "Arsenic+Phosphorus-Boron" ;# Create and select a data field using  
                                      ;# solution variables  
select z= log10(BActive)      ;# Create and select a data field from  
                                      ;# the active boron concentration
```

The list of available data fields can be retrieved by using `select list`. The name that can appear in the expression of the `z` parameter can be either a data field or a term.

A term is defined with the `term` command and is also an expression containing solution variables, data fields, constants, and so on (see [term on page 1232](#)). Numerous terms are created automatically in the `diffuse` command (see [diffuse on page 935](#)) and any of these terms can be selected.

When a data field is selected (or created and selected) with the `select` command, the data field can be viewed or operated on. The following commands can operate on the selected field: `interpolate`, `layers`, `plot.1d`, `print.1d`, `print.data`, and `slice`.

---

## Obtaining 1D Data Cuts

After a `select` command has been issued, you can obtain 1D cuts through the data along one of the principal axes using the `slice` or `print.1d` command. The `slice` command returns a list of coordinate data pairs. To make a cut perpendicular to *x*, specify the `x` parameter, similarly for *y* and *z*.

The `print.1d` command returns a list of data-point lists. Each data-point list contains the coordinate, data value, and the material name at that coordinate. Again, a cut perpendicular to *x* is made by specifying the `x` parameter and, similarly, for the *y* and *z* cuts.

The `plot.1d` command can be used to view profiles with a temporary X11 graphics tool.

---

## Examples

Sentaurus Process can run in interactive mode if there is no command file given on the command line. In this case, you are prompted with the `sprocess>` prompt for commands. If a command file is given, commands are read from this file. In interactive mode, the return value of the commands is always displayed. You can set variables to the return value of a command by using the syntax:

```
set var [command]
```

In this case, `command` is executed and a Tcl variable `var` is created if it does not already exist, and the value of `var` is set to the return value of `command`. In addition, the return value of `command` is displayed. It is also possible to write the return value to a user-defined file. The following examples demonstrate the differences and functionality of the `slice` and `print.1d` commands:

```
sprocess> select z= Vacancy
sprocess> slice y=0.6
{-1.000000e-02 4.804720e+16
-9.340278e-03 5.869015e+16}
```

## 14: Extracting Results

### Examples

```
...
0.000000e+00 5.969905e+17
0.000000e+00 7.075867e+17
7.421875e-04 7.618894e+17

...
sprocess> print.1d y=0.6
{ Distance Value Material }
{ -1.00000e-02 4.80472e+16 Oxide }
{ -9.34028e-03 5.86902e+16 Oxide }

...
{ 0.00000e+00 5.96991e+17 Oxide }
{ 0.00000e+00 7.07587e+17 Silicon }
{ 7.42188e-04 7.61889e+17 Silicon }

...
```

Here, the `slice` command returns raw coordinate data pairs, whereas `print.1d` returns a header and coordinate data–material triplets. In both cases, the coordinates are given in micrometers and the concentration is in  $\text{cm}^{-3}$ .

To illustrate how data from these functions can be manipulated with Tcl, suppose you require a 1D profile of Vacancy, which starts with 0.0 as the first coordinate, and the Vacancy concentration to be in  $\mu\text{m}^{-3}$ .

First, create a Tcl list from the data returned by the slice, and convert data in that list to a new list, such as:

```
set myList [lindex [slice y=0.6] 0]          ;# Create a new list from slice
                                              # command called myList
set offset [lindex myList 0]                  ;# Grab the offset, that is, the
                                              # first coordinate
list modList                                ;# Create new Tcl list where
                                              # modified data will reside
foreach { coord data } $myList { \
    lappend modList [expr $coord-$offset]   ;# Convert coordinate by subtracting
                                              # the offset and append to modList
    lappend modList [expr $data*1.0e-12]    ;# Convert data to  $\mu\text{m}^{-3}$  units and
                                              # append to modList
}
}
```

The above example uses the following Tcl commands:

- `lindex` retrieves a given element of a list.
- `list` creates a list.
- `lappend` appends an element to the end of a list.
- `expr` evaluates a math expression.
- `foreach` is used for looping.

For example, to write modList to a file called `xy.dat`:

```
set fileID [open xy.dat w] ;# Use the Tcl open command
                           # to open a file for writing
foreach { x y } $modList { puts $fileID "$x $y" } ;# Write modList line by line
close $fileID
```

## Determining the Dose: Layers

The `layers` command computes the dose of the selected data field along one of the principal axes. The syntax to specify the cut is the same as the `slice` command (see [slice on page 1199](#)). As with the other commands, the information is returned as a list of lists:

```
sprocess> sel z= Vacancy
sprocess> set layerInfo [layers y=0.5]; # For a 2d structure,
           either x or y must be specified
{
    Top      Bottom      Integral   Material}
{-2.06000e-01 -6.00000e-03 9.98843e+14 Silicon}
{-6.00000e-03 0.00000e+00 3.97970e+09 Oxide)
{ 0.00000e+00 1.00000e+00 2.81858e+05 PolySilicon}
```

The top and bottom coordinates are in micrometers. To obtain the total integrated dose along  $y=0.5$ , use:

```
sprocess> set total 0
0
# Loop over layerInfo list of lists skipping header list,
# and retrieve the 3rd element of each list (first element has 0 index)
# which corresponds to the Integral for that layer.
sprocess> for { set i 1 } { $i < [llength $layerInfo] } { incr i } {
>     set total [expr $total + [lindex [lindex $layerInfo $i] 2]]
> }
sprocess> puts $total
9.991288377e+14
sprocess>
```

In addition to the Tcl commands used in the previous section, this example uses the following:

- `llength` returns the size of a given list.
- `incr` increases an integer by 1.

For more information about the `layers` command, see [layers on page 1051](#).

## 14: Extracting Results

Extracting Values and Level Crossings: interpolate

---

# Extracting Values and Level Crossings: interpolate

The `interpolate` command has two purposes: to obtain the position at which a profile crosses a particular value and to retrieve a value at a particular location in space. Interpolation is used to accomplish both tasks.

The main arguments of this command are `value`, `x`, `y`, and `z`. The combination of these arguments determines how the command operates on a selected data field:

- In 1D simulations, you must supply either `x` or `value`. If `x` is supplied, Sentaurus Process returns the value at `x`. If `value` is supplied, Sentaurus Process returns the locations at which the selected profile crosses `value`.
- In 2D simulations, two of these arguments must be given (not `z`).
- In 3D simulations, three of these arguments must be given.

For example, in 2D simulations, if `x` and `value` are given, the locations along `x` where `value` is crossed are returned. If `x` and `y` are given, the value at this location is returned.

For more information, see [interpolate on page 1033](#).

---

# Extracting Values During diffuse Step: extract

The `extract` command is used to extract historical data during diffuse steps. This command allows you to define the data extraction script with the `command` parameter. The extraction script is composed typically of the `select` command for choosing the data field for extraction and the `interpolate` command for retrieving the value at a specified location. Only values returned by the `interpolate` command, at each time step, are stored in the historical data values.

For example, to extract the boron concentration at position 0.04  $\mu\text{m}$  in the silicon and the YY component of the element stress at position -0.001  $\mu\text{m}$  in the oxide for each diffuse substep:

```
extract name=etest command= {
    sel z=Boron
    interpolate Silicon x=0.04
    sel z=StressEL_yy element
    interpolate Oxide x=-0.001
}
```

This command must be defined before the `diffuse` step. After the `diffuse` steps of interest, the following command retrieves the extracted data values for the defined extraction `etest`:

```
extract name=etest print
```

The values are returned as a Tcl list with the format:

```
<time1> <Boron1> <Syy1> <time2> <Boron2> <Syy2> ...
```

The following script demonstrates how to manipulate this list for more formatted output:

```
set extdata [extract name=etest print]
foreach { time bval sval } $extdata {
    puts "$time $bval $sval"
}
```

Output from the above script is:

```
0.000000e+00 4.738727e+15 6.000000e+09
1.000000e-04 4.738727e+15 4.793201e+09
2.503231e-04 4.738727e+15 4.793201e+09
5.509694e-04 4.738727e+15 4.793201e+09
1.152262e-03 4.738727e+15 4.793201e+09
...
...
```

For more information, see [extract on page 960](#).

---

## Optimizing Parameters Automatically

Previously, users relied on the Optimizer tool in Sentaurus Workbench to perform parameter optimization. Sentaurus Process provides a built-in capability for automatic optimization of parameters using the `optimize` command (see [optimize on page 1090](#)).

To use this feature, a Tcl procedure must be created that takes as input the current values of the parameters to be optimized, and returns a corresponding result. Although writing the procedure is a small extra task for users, this design allows greater flexibility in the types of optimization that can be performed. The procedure can specify anything from a simple analytic function to a complete process simulation flow. The form of the result is a vector of values from which an error is computed based on user-defined target data. This generic flow allows for various applications (such as dopant profiles resulting from multiple process steps or the thickness of an oxide layer).

To use the automatic parameter optimization feature, the Tcl procedure is introduced into an input file or sourced from an external file before calling the `optimize` command.

## 14: Extracting Results

### Fitting Routines

The `optimize` command also allows you to weigh target values, to log the history of optimization steps, and to specify the maximum number of iterations and other convergence criteria.

---

## Fitting Routines

The following commands provide fitting capabilities.

---

### FitArrhenius Command

This command is used to find the best prefactor and energy for an Arrhenius fit of a given profile, for example:

```
sprocess> list dat          ;# This is the list to be passed to FitArrhenius
sprocess> foreach temp { 700 800 900 1000 } {
  > SetTemp $temp
  > lappend dat $temp      ;# dat will contain "temp" - "Arrhenius val" pairs
  > lappend dat [Arrhenius 0.1 1.0];      ;# Arrhenius takes prefactor and
                                             # activation energy
}
sprocess> FitArrhenius $dat          ;# Send the list to FitArrhenius
0.0999999308634 1.00030363776 -0.999999999866 ;# Return prefactor, energy
                                                    ;# and corr factor
sprocess>
```

This command takes a list of temperature–function pairs. The unit of temperature is degree Celsius. The return value is a list where the first member is the prefactor, the second member is the activation energy [eV], and the third member is the correlation factor. Absolute values of the correlation factor close to one are desirable.

---

### FitLine Command

This command is used to find the best offset and slope for a given set of data, for example:

```
sprocess> foreach temp { 700 800 900 1000 } {
  > lappend dat $temp
  > lappend dat [expr 110 + 10*$temp]
}
sprocess> FitLine $dat          ;# Get the slope, offset, and correlation factor
10.0 110.0 1.0
```

---

## FitPearson Command

This command is used to extract the best Pearson parameters of a profile.

---

## FitPearsonFloor Command

This command is a modification of the `FitPearson` command and is used to set a floor for the data value so that only data points with values greater than the given floor are used for the Pearson fit.

An example of using this command is one that contains the command `PearsonProfile`, which can be called to create a Pearson–IV, Pearson–V, or Pearson–VI profile depending on the parameters sent. It takes as its arguments the name of the data field to be created and a list of parameters in this order: dose [ $\text{cm}^{-2}$ ], projected range, standard deviation, skewness, and kurtosis. `FitPearsonFloor` takes the minimum value and a list of  $x$   $y$  values, which are to be fit to a Pearson. It returns parameters in the same order as the list of parameters for `PearsonProfile`:

```
sprocess> PearsonProfile Arsenic {1e14 0.0650 0.0228 0.577 3.4390}
                                ;# Corresponds to 100 keV As implant
sprocess> select z= Arsenic
sprocess> FitPearsonFloor 1.0e10 [lindex [slice silicon] 0]
9.99999659675e+13 0.0649998507454 0.0227994405041 0.576718866676
3.4368839917
sprocess>
```

---

## Resistivity

The background concentration of the wafer can be defined using the resistivity of the wafer. You can define the resistivity of the wafer with the `init` command, which requires a field name to calculate the background concentration. For example:

```
line x location = 0 tag=top
line x location = 10 tag=bottom
region silicon xlo = top xhi = bottom
init field=boron silicon resistivity=1.4
```

sets the boron concentration of the wafer to  $1.08 \times 10^{16} \text{ cm}^{-3}$  in silicon.

The resistivity is given in  $\Omega\text{cm}$ , and the resistivity is calculated by:

$$RHO = (qN\mu)^{-1} \quad (996)$$

## 14: Extracting Results

### Resistivity

where:

- $q$  is the electron density.
- $N$  is the background concentration.
- $\mu$  is the mobility.

The mobility model can be selected using the command:

```
pdbSet <material> <dopant> Mobility.Model <model>
```

where <model> can be:

- Model1 [1]:

$$\mu = \mu_{\min} + \frac{\mu_{\max} - \mu_{\min}}{1 + \left(\frac{N}{N_r}\right)^\alpha} \quad (997)$$

- Model2 [2]:

$$\mu = \mu_{\min} e^{-\left(\frac{P_C}{N}\right)} + \frac{\mu_{\max} - \mu_{\min2}}{1 + \left(\frac{N}{N_r}\right)^\alpha} - \frac{\mu_m}{1 + \left(\frac{N_s}{N}\right)^\beta} \quad (998)$$

- Model3 [3]:

$$\begin{aligned} \mu_p &= \mu_{\min} e^{-\left(\frac{P_C}{N}\right)} + \frac{\mu_{\max}}{1 + \left(\frac{N}{N_r}\right)^\alpha} \\ \mu_n &= 10^{\frac{A_0 + A_1 X + A_2 X^2 + A_3 X^3}{1 + B_1 X + B_2 X^2 + B_3 X^3}} \\ X &= \log\left(\frac{N}{N_r}\right) \end{aligned} \quad (999)$$

where  $N_r$ ,  $\mu_{\min}$ ,  $\mu_{\min2}$ ,  $\mu_{\max}$ ,  $\mu_m$ ,  $P_C$ ,  $A_0$ ,  $A_1$ ,  $A_2$ ,  $A_3$ ,  $B_1$ ,  $B_2$ ,  $B_3$ ,  $\beta$ , and  $\alpha$  are fitting parameters for the empirical formulas.

The fitting parameters can be set using the following commands:

```
pdbSet <material> <dopant> uMin {<n>}
pdbSet <material> <dopant> uMin2 {<n>}
pdbSet <material> <dopant> uMax {<n>}
pdbSet <material> <dopant> uM {<n>}
pdbSet <material> <dopant> uNr {<n>}
pdbSet <material> <dopant> uNs {<n>}
pdbSet <material> <dopant> uPC {<n>}
```

```

pdbSet <material> <dopant> uBeta {<n>}
pdbSet <material> <dopant> uAlpha {<n>}
pdbSet <material> <dopant> A0 {<n>}
pdbSet <material> <dopant> A1 {<n>}
pdbSet <material> <dopant> A2 {<n>}
pdbSet <material> <dopant> A3 {<n>}
pdbSet <material> <dopant> B1 {<n>}
pdbSet <material> <dopant> B2 {<n>}
pdbSet <material> <dopant> B3 {<n>}

```

In addition to these models, a user-defined mobility model can be set using the command:

```
pdbSet <material> <dopant> Mobility.Equation <String Expression>
```

For example, the `Mobility1` model for boron in silicon can be set using:

```

pdbSet Silicon Boron Mobility.Equation \
  "(49.705+(467.729-49.705)/(1+abs(tNetActive/1.606e+17)^0.7))"

```

`tNetActive` is the internal name for  $N$ .

**NOTE** To change the model and default model parameters, use the `setMobilityModel` command (see [setMobilityModel on page 1181](#)).

## Sheet Resistance

The sheet resistance and the p-n junction depth of a semiconductor layer in the vertical direction are calculated using the command (see [SheetResistance on page 1193](#)):

```
SheetResistance [x=<n>] [y=<n>] [z=<n>]
```

For example, in 3D simulations, two axes must be specified:

```
SheetResistance y=0.4 z=-0.1
```

The sheet resistance formula is given by:

$$R_s = \frac{1}{\frac{\int_{pn_i} q(\mu_n n + \mu_p p) dx}{pn_i}} \quad (1000)$$

where  $\mu_x$  is the mobility of holes ( $p$ ) or electrons ( $n$ ) given in [Eq. 997](#), or [Eq. 998](#), or [Eq. 999](#). The active concentration of dopants is calculated at the last diffusion temperature. The electron ( $n$ ) and hole ( $p$ ) concentrations are calculated assuming charge neutrality at a temperature of 300 K.

## 14: Extracting Results

### References

Sheet resistance can be calculated only after a `diffuse` command or an activation step, for example:

```
diffuse time=0.0 temperatur=1000
SheetResistance y=9.4 z=-0.1
```

Since not all data fields are stored in the TDR file, the sheet resistance may not be calculated after loading the TDR file even though the last command was a `diffuse` command.

---

## References

- [1] D. A. Antoniadis, A. G. Gonzalez, and R. W. Dutton, “Boron in Near-Intrinsic <100> and <111> Silicon under Inert and Oxidizing Ambients—Diffusion and Segregation,” *Journal of the Electrochemical Society*, vol. 125, no. 5, pp. 813–819, 1978.
- [2] G. Masetti, M. Severi, and S. Solmi, “Modeling of Carrier Mobility Against Carrier Concentration in Arsenic-, Phosphorus-, and Boron-Doped Silicon,” *IEEE Transactions on Electron Devices*, vol. ED-30, no. 7, pp. 764–769, 1983.
- [3] W. R. Thurber *et al.*, *The Relationship Between Resistivity and Dopant Density for Phosphorus- and Boron-Doped Silicon*, National Bureau of Standards Special Publication 400-64, Washington, DC, USA, May 1981.

# CHAPTER 15 Numerics

---

*This chapter discusses numerics-related issues, time integration methods, and the linear solvers used in Sentaurus Process.*

## Overview

In Sentaurus Process, during the simulation of diffusion steps, different sets of nonlinear partial differential equations must be solved:

- Oxidant diffusion and reaction
- Dopant diffusion and reaction
- Stress equations

In the case of silicidation, the transport and reactions of dissolved silicon or dissolved metal is handled similar to the oxidant diffusion and reaction.

The oxidant, dopant, and point-defect equations are solved on the simulation mesh using a trapezoidal rule/backward differentiation formula (TRBDF) time discretization, a finite volume (box) method for the spatial integration, and a Newton method to solve the nonlinear equations.

For the discretization of the nonlinear stress equations, piecewise linear finite elements are used. If stress history is tracked, the stress equations are solved, not only during the simulation of diffusion steps, but also at the end of etch and deposit steps.

Various direct and iterative solvers are integrated in Sentaurus Process to solve the large systems of linear equations in each Newton iteration. By default, for all equations in 1D simulations and for mechanics equations in 2D simulations, the parallel direct solver PARDISO is used. For diffusion equations in two dimensions and for all equations in three dimensions, the iterative solver ILS is used. The solver can be selected using the `math` command:

```
math ils
```

This command selects the solver ILS for all types of equation in 1D, 2D, and 3D. Separate selections can be made for the various spatial dimensions and for the solution of mechanics equations and diffusion equations (the same settings are used for both oxidant and dopant–point defect equations).

## 15: Numerics

### Setting Parameters of the Iterative Solver ILS

The parameters `Flow` and `diffuse` select the type of equation, and the parameter `dim` specifies the spatial dimension:

```
math Flow    dim=2 ils
math diffuse dim=2 pardiso
math Flow    dim=3 pardiso
```

If a direct solver is used, a modified Newton method is used by default; Sentaurus Process tries to avoid the recomputation and factorization of a new matrix and will reuse the last factorized matrix, as long as the convergence rate remains sufficiently high. For the iterative solvers, by default, a modified Newton scheme is used as well.

The `math` command is used to specify various parameters for the Newton iterations and to define resources and specifications for the linear solvers (see [math on page 1073](#)).

For the default settings for ILS, refer to the Parameter Database (PDB). More detailed settings for ILS can be made using `pdbSet` commands as described in the next section.

---

## Setting Parameters of the Iterative Solver ILS

The iterative solver ILS is used by default to solve the linear systems for `diffuse` in 2D simulations and for both `Flow` and `diffuse` in 3D simulations. Default parameters for ILS have been added to the parameter database. To specify modified parameters for ILS, such as the type of iterative scheme, the number of iterations, the output verbosity, or the memory resources, use the `pdbSet` commands.

**NOTE** In the `pdbSet` commands, parameters must be specified separately for each type of problem (`Flow` or `diffuse`) and for each dimension (1D, 2D, or 3D).

**NOTE** ILS is not recommended for use in 1D simulations because of the simple structure of matrices arising in 1D cases. The default direct solver PARDISO is the correct choice for 1D simulations.

Different ILS parameters can be specified for `diffuse` and `Flow`, both in 2D or 3D. In general, the `pdbSet` command for the ILS parameters has the form:

```
pdbSet Math [diffuse | Flow] [2D | 3D] ILS.[command] [value]
```

The following ILS commands are available:

<code>ILS.compact</code>	Boolean
<code>ILS.fgmres.restart</code>	Double
<code>ILS.gmres.restart</code>	Double
<code>ILS.fit</code>	Double

ILS.ilut.tau	Double
ILS.leftPreconditioner	Boolean
ILS.maxit	Double
ILS.method	String
ILS.nonsymmOrdering	String
ILS.okayForModNewton	Boolean
ILS.preconditioner	String
ILS.recompute.ordering	Double
ILS.refine.residual	Double
ILS.refine.iterate	Double
ILS.scaling	String
ILS.symmOrdering	String
ILS.tolabs	Double
ILS.tolrel	Double
ILS.tolunprec	Double
ILS.useILSRCFile	Boolean
ILS.verbose	Double

To select the GMRES method, for example, `gmres(60)`, use:

```
pdbSet Math diffuse 3D ILS.method      gmres
pdbSet Math diffuse 3D ILS.gmres.restart 60
```

To specify the FlexibleGMRES method, for example, `fgmres(40)`, to solve the stress equations, use:

```
pdbSet Math Flow 3D ILS.method      fgmres
pdbSet Math Flow 3D ILS.fgmres.restart 40
pdbSet Math Flow 3D ILS.fit      5
```

To select the efficient reuse mode (on each 3D diffuse time step, the costly reordering is applied only once to a first Jacobian system), specify:

```
pdbSet Math diffuse 3D ILS.recompute.ordering 2
```

and to return to reordering for every system, use:

```
pdbSet Math diffuse 3D ILS.recompute.ordering 1
```

To improve the accuracy and convergence of iterative linear solvers, use an enhanced option by specifying (default value is 0):

```
pdbSet Math [diffuse | Flow] [2D | 3D] ILS.refine.iterate 1
```

The 3D diffusion `gmres` solver with the most advanced parallel implementation is used by default. The advanced parallel implementation is activated using:

```
pdbSet Math diffuse 3D ILS.hpc.mode 4
```

## 15: Numerics

### Setting Parameters of the Iterative Solver ILS

where:

- A value of 4 activates algorithmic improvements made in Versions N-2017.09, M-2016.12, L-2016.03, K-2015.06, and J-2014.09. This is the default behavior in Versions N-2017.09, M-2016.12, and L-2016.03.
- A value of 3 corresponds to Versions I-2013.12 and H-2013.03.
- A value of 2 corresponds to Versions G-2012.06 and F-2011.09.
- A value of 1 was introduced in Version E-2010.12.

To deactivate this option, use:

```
pdbSet Math diffuse 3D ILS.hpc.mode 0
```

To select the solvers for mechanics, STS2 or STCG2 for 2D, and STS3 or STCG3 for 3D, for example, `sts3`, use:

```
pdbSet Math Flow 3D ILS.method      sts3
pdbSet Math Flow 3D ILS.tolrel      1e-10
pdbSet Math Flow 3D ILS.ilut.tau    5e-4
pdbSet Math Flow 3D ILS.scaling     diagsym
pdbSet Math Flow 3D ILS.nonsymmOrdering  none
```

For the mechanics solvers STS2, STS3, STCG2, and STCG3, it is mandatory to specify `ILS.scaling` as `diagsym`, and `ILS.nonsymmOrdering` as `none`. It is also recommended to specify the value for the parameter `ILS.ilut.tau` in the range of  $5 \times 10^{-4} - 5 \times 10^{-5}$ .

To improve convergence of the mechanics solver STS2 or STS3, use an enhanced version of the solver by specifying, respectively (default value is 0):

```
pdbSet Math Flow 2D ILS.refine.sts 1
```

or:

```
pdbSet Math Flow 3D ILS.refine.sts 1
```

The enhanced version takes advantage of results from previous solve steps, so the actual performance gain can vary depending on the simulation setup, and it performs best when there is a sequence of mechanical solve steps, as in temperature ramps.

To active the STS solver which improves robustness and speed, use:

```
pdbSet Math Flow 3D ILS.refine.sts 2
```

---

## Partitioning and Parallel Matrix Assembly

Sentaurus Process can assemble the diffusion and mechanics matrices in parallel on multicore machines. To switch on the parallel assembly, use:

```
math numThreads=<i> | numThreadsAssembly=<i>
```

where numThreads is the number of threads that would be used during the matrix assembly. numThreads is a general keyword (see [math on page 1073](#)) used by both implantation and linear solvers. If you want to use a different number of threads for diffusion matrix assembly, use the keyword numThreadsAssembly. If the number of threads is greater than 1, Sentaurus Process first creates the threads.

To modify the thread stack size, use:

```
math threadStackSize=<i>
```

**NOTE** Parallel assembly of the matrix is performed only for inert anneals. It is recommended that numThreadsAssembly does not exceed the number of actual cores of the computer. Parallel assembly of the matrix is not available for moving-boundary problems such as oxidation and silicidation.

Sentaurus Process then partitions the mesh structure into levels, and each level is divided into different domains at the beginning of the diffusion step. For example, [Figure 156 on page 888](#) shows a structure with three levels. The first level (blue) (L0) has four domains: D0, D1, D2, and D3. Elements belonging to each domain on the same level do not cross over to the other domains. The second level (orange) (L1) also has four domains: D0, D1, D2, and D3. Again, the elements on the same level do not cross over to the other domains. The third level (green) (L2) has only one domain: D0. This is the last level and contains all the elements not included in the previous levels.

To control the partitioning, use:

```
math maxNumberOfDomains=<i> | NumberOfElementsPerDomain=<i>
```

**NOTE** The maxNumberOfDomains argument is the maximum number of domains that each level of partition can have. It is recommended that maxNumberOfDomains is equal to or greater than the number of threads used. The argument NumberOfElementsPerDomain is the number of elements that should go to each domain.

## 15: Numerics

### Partitioning and Parallel Matrix Assembly

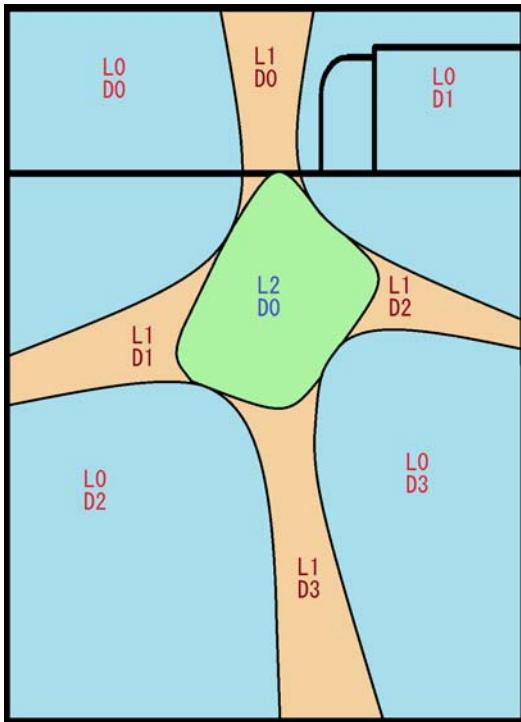


Figure 156 Partitioned mesh structure

The final number of domains at each level is determined by:

$$\text{domains} = \min(\text{maxNumberOfDomains}, \frac{\text{Number of Edges}}{\text{NumberOfElementsPerDomain}}) \quad (1001)$$

To partition the mesh, based on material type, give weight to each material using the command:

```
pdbSet <material> PartitionWeight <n>
```

For example:

```
pdbSet Silicon PartitionWeight 10  
pdbSet Gas PartitionWeight 0
```

gives more weight to silicon mesh elements than the gas mesh elements during partitioning. This allows Sentaurus Process to distribute the work among the threads more evenly since there is no matrix assembly for the gas mesh.

Partition weights for mechanics assembly can be specified separately with:

```
pdbSet <material> Mechanics PartitionWeight <n>
```

This allows balancing the workload among threads according to the stress analysis methods for different material behaviors. If the partition weights for mechanics assembly are not defined, the partition weights for diffusion assembly are used by default.

---

## Matrix Size Manipulation

The size of the matrix used during diffusion assembly is automatically determined based on the number of solution variables and nodes in the structure. In most cases the allocated matrix size is more than sufficient. If the matrix size becomes insufficient during the assembly, the matrix size will be increased automatically by 10%. You can change the default 10% value by using the command:

```
pdbSet Math Matrix.Size.Scale <n>
```

where the value <n> should be greater than one.

You also can increase the automatically determined matrix size using the command:

```
pdbSet Math Assembly.Matrix.Size.Scale <n>
```

where the value <n> should be greater than one.

**NOTE** Be careful when choosing the matrix scaling values because it can exhaust the computer memory for large scaling values.

---

## Node and Equation Ordering

Because the order of nodes in meshes does not follow a specific order by default, adjacent nodes may be far from each other in the internal node list. The order may not have much effect on simulation time for small examples (such as 2D), but it may degrade 3D results. The nodes in the structure can be ordered meshwise or globally using the command:

```
pdbSet Math <1D | 2D | 3D> Reorder.Nodes <model>
```

where <model> is None (default), Mesh, or Global.

The default order of equation numbering in the structure is based on the meshes. Each node in the mesh receives an equation number from a solution variable and the same is repeated for the next solution. This may create many distributed entries in the assembly matrix. Again, the order may not greatly affect the simulation time for small examples (such as 2D), but it may degrade 3D results. It is possible to number equations based on solutions by taking a node in the mesh, numbering it for each solution variable, and moving to the next node in the mesh. This creates

better-distributed entries in the assembly matrix. The order can be changed using the command:

```
pdbSet Math <1D | 2D | 3D> Reorder.Equations <model>
```

where <model> is None (default) or Solution.

---

## Time Integration

The TRBDF method [1] is used for time integration by default for time-dependent problems. It also is possible to choose the backward Euler method for the time integration. The following command can be used to switch between methods:

```
math [tr_bdf | euler]
```

A TRBDF integration step consists of a trapezoidal step followed by a backward difference step. A second trapezoidal solution is used to estimate the local truncation error and to determine the size of the next time step.

The local truncation error can be estimated by either a Milne's device (the default method) or the divided difference method. The following command switches between methods:

```
math [milne | difference]
```

The local truncation error for the next time-step estimation can be modified using the command:

```
pdbSet Math Time.Step.Function {<model>}
```

where <model> is Damped, UnDamped, or Linear. The Damped model applies a logarithmic damping function to the truncation error if the error is greater than 1.0. The UnDamped model does not modify the error. The Linear model applies a linear damping function to the truncation error if the error is greater than 1.0. The Linear model matches that of TSUPREM-4.

When the geometry of a simulation structure evolves, one cycle of the TRBDF time integration requires the geometric coefficients at three incidents, that is,  $t = t_0, t_0 + \Delta t_{TR}, t_0 + \Delta t$ . To reduce the computational time to calculate the geometric coefficients, especially in three dimensions, the geometric coefficients at  $t = t_0 + \Delta t_{TR}$  can be set to the interpolated values by assuming that the coefficients change linearly during  $\Delta t$ , which reduces the number of the box method calls by one third:

```
pdbSet Math 3D Use.Interpolated.G geom.Coeff 1
```

or:

```
math dimension=3 use.interpolated.geom.coeff
```

## Time-Step Control

This section discussed different time-step controls.

### Time-Step Control for PDEs

Sentaurus Process provides automatic time-step control. You can modify some of the control parameters.

The first time step of the `diffuse` command uses the initial time given with the `diffuse` command (see [diffuse on page 935](#)).

In an ideal situation, oxidation, mechanics, and diffusion time steps are equal to each other, and the next time step is increased by the `IncreaseRatio`:

$$t_{n+1} = I_{\text{ratio}} t_n \quad (1002)$$

where  $t_{n+1}$  is the next diffusion time step,  $t_n$  is the current time step, and  $I_{\text{ratio}}$  is the `IncreaseRatio`. The default for `IncreaseRatio` is 2.

Use the following command to change `IncreaseRatio`:

```
pdbSet Diffuse IncreaseRatio {<n>}
```

In some cases, the ideal time step can be solution limited, grid limited, or reduced:

- *Solution limited* is the case when the time step is shortened to decrease the local truncation error; in a log file, such steps are marked by (s).
- *Grid limited* is the case when the time step is reduced because of a grid motion; in a log file, such steps are marked by (g).
- *Reduced* is the case when the time step is reduced to prevent overstepping of oxidation or mechanics steps; in log files, such steps are marked by (r).

If convergence is not achieved, the next time step is reduced by the `ReduceRatio`:

$$\tilde{t}_{n+1} = R_{\text{ratio}} t_{n+1} \quad (1003)$$

The following command can be used to change ReduceRatio:

```
pdbSet Diffuse ReduceRatio {<n>}
```

For more information about the convergence during diffusion, use the command:

```
pdbSet Diffuse Convergence.Info <1 | 0>
```

Typical output with information level=2 will look like:

```
Iter Potential Boron Arsenic Int Vac B4
1 4.345e-02 2.244e+01 2.512e+00 5.096e+03 1.835e+02 2.599e-06
-- -- -- -- -- -- -- -- -- -- -- -- -- -- -- --
Mesh: bulk Mater: Silicon
Org. Val. Org. Updt. Org.-Updt Apld. Updt. Error Location
Boron 5.7e+18 1.8e+17 5.5e+18 5.5e+18 3.1e+02 (4.82e-01 1.0e+00 1.00e+00) (UCS)
(1.00e+00 1.0e+00 -4.82e-01) (DFISE)
Arsenic 7.2e+16 3.1e+14 7.2e+16 7.2e+16 4.3e+01 (4.82e-01 1.0e+00 1.00e+00) (UCS)
(1.00e+00 1.0e+00 -4.82e-01) (DFISE)
Int 2.8e+12 -1.3e+13 1.5e+13 1.5e+13 4.5e+04 (4.82e-01 1.0e+00 1.00e+00) (UCS)
(1.00e+00 1.0e+00 -4.82e-01) (DFISE)
Vac 3.5e+14 5.5e+13 2.9e+14 2.9e+14 1.5e+03 (4.82e-01 1.0e+00 1.00e+00) (UCS)
(1.00e+00 1.0e+00 -4.82e-01) (DFISE)
Largest update: Int in Silicon @ (5.01e-01 1.00e+00 1.00e+00) (UCS)
(1.00e+00 1.00e+00 -5.01e-01) (DFISE)
```

where:

- Org.Val is the original value at the node.
- Org.Updt is the original update at the node.
- Org.-Updt is the Original Value – Original Update.
- Apld. Updt. is the applied update.
- Location is the location (in  $\mu\text{m}$ ) of the node in both the unified coordinate system (UCS) and the DF-ISE coordinate system.

Different time-step control models are available:

- Two history-based models involving all previous time steps within the diffuse command: BPTS and NGLTS.

BPTS uses the *biggest previous time step* from the history, such that Eq. 1002 is modified as:

$$t_{n+1} = I_{\text{ratio}} t_{\text{BPTS}, n} \quad (1004)$$

NGLTS uses the latest *nongrid limited time step*, and Eq. 1002 is modified as:

$$t_{n+1} = I_{\text{ratio}} t_{\text{NGLTS}, n} \quad (1005)$$

Use the following command to choose the time-step control model:

```
pdbSet Compute TSEM <model>
```

where <model> can be None, BPTS, or NGLTS.

## Error Control for PDEs

To control errors during transient simulation, Sentaurus Process uses the following to calculate the error:

$$e = \left( \frac{1}{N} \sum_{i=1}^N \left( \frac{|u_i|}{|\text{sol}_i| \times \text{TransRelErr} + \text{AbsErr}} \right)^2 \right)^{1/2} \quad (1006)$$

where the sum is taken over all solution variables, and  $u_i$  is the update for solution  $\text{sol}_i$ . TransRelErr and AbsErr are the transient relative error and absolute error for the solution variables, respectively. They can be set using the commands:

```
pdbSetDouble <mater> <solution> Transient.Rel.Error <n>
pdbSetDouble <mater> <solution> Abs.Error <n>
```

where <mater> is the material name.

To control errors during nonlinear Newton iterations, Sentaurus Process uses the following to calculate the error:

$$e = \left( \frac{1}{N} \sum_{i=1}^N \left( \frac{|u_i|}{|\text{sol}_i| \times \text{RelErr} + \text{AbsErr}} \right)^2 \right)^{1/2} \quad (1007)$$

where RelErr is the relative error for the solution variables. It can be set using the command:

```
pdbSetDouble <mater> <solution> Rel.Error <n>
```

**NOTE** If the error control parameter is not defined in the PDB for a material or a solution, the long-hand command `pdbSetDouble` must be used.

## Time-Step Control for Mechanics

Automatic time-step control for mechanics is activated only if the structure contains certain nonlinear features that require Newton iterations. The size of the time step is adjusted based on satisfaction of certain convergence criteria.

## Convergence Criteria

To check the convergence of Newton iterations for mechanics equations [2][3], the criteria are:

- Force residual
- Energy
- Displacement

The force residual criterion checks the satisfaction of force equilibrium by comparing the maximum norm of the residual ( $R = F^{\text{external}} - F^{\text{internal}}$ ) against a reference value:

$$\|R_{n+1}^i\|_\infty \leq \varepsilon_R \|R_{n+1}^{-1}\| \quad (1008)$$

The reference value of the force residual is computed automatically by taking a norm of the element force residual vector at the first Newton iteration in a time step.

The energy criterion checks the satisfaction of the minimization of energy at equilibrium by comparing the change in energy against a reference value:

$$\sqrt{\|\Delta u_{n+1}^i \cdot R_{n+1}^i\|} \leq \varepsilon_E \sqrt{\|\Delta u_n \cdot R_{n+1}^1\|} \quad (1009)$$

The reference value of energy is computed automatically by taking a dot product of the force residual and the displacement increment ( $\Delta u = v\Delta t$ ) vector at the first Newton iteration in a time step.

The displacement criterion checks the satisfaction of the solution accuracy by comparing the maximum norm of the displacement increment against a reference value:

$$\|\Delta u_{n+1}^i\|_\infty \leq \varepsilon_u \|\Delta u_n\| \quad (1010)$$

The reference value of displacement is computed automatically by taking a norm of the displacement increment vector at the start of the first Newton iteration in a time step.

The force residual and the energy criteria are checked by default. Optionally, the energy criterion may be replaced by the displacement criterion. Use the following parameters to activate or deactivate any of the convergence criteria:

```

pdbSet Mechanics Convergence.Force.Check <n>
pdbSet Mechanics Convergence.Energy.Check <n>
pdbSet Mechanics Convergence.Displacement.Check <n>
```

where  $<n>$  is either 0 (deactivate) or 1 (activate).

The choices for the force residual and the displacement reference value norms that can be set using the following command are:

```
pdbSet Mechanics Convergence.Check.Norm [RMS | ABS]
```

where RMS refers to the root mean square value (default) and ABS refers to the mean absolute value.

The reference values for any of the convergence criteria can be changed by using the commands:

```
pdbSet Mechanics Convergence.Force.RefVal <n>
pdbSet Mechanics Convergence.Energy.RefVal <n>
pdbSet Mechanics Convergence.Displacement.RefVal <n>
```

where <n> is a suitable positive value.

By default, the tolerance for each of the convergence criteria is set to 0.001 and can be changed by using the commands:

```
pdbSet Mechanics Convergence.Force.Tolerance <n>
pdbSet Mechanics Convergence.Energy.Tolerance <n>
pdbSet Mechanics Convergence.Displacement.Tolerance <n>
```

where <n> is a value between 0.0 and 1.0.

Convergence criteria are checked in every iteration until either they are satisfied or the maximum number of Newton iterations is reached. The default value for the maximum number of Newton iteration is 8, and this can be changed using the command:

```
pdbSet Mechanics MaxIterations <n>
```

where <n> is a value greater than zero.

## Time-Step Cutback

An automatic time-step cutback procedure interrupts the Newton iteration loop and restarts the time step with a smaller size when any of the following issues is encountered:

- Convergence criteria are not satisfied within the maximum number of Newton iterations.
- The solution converges very slowly over several iterations.
- The solution diverges over several iterations.

To check convergence details during solve steps, specify `info=1` in the `solve` command.

## 15: Numerics

### References

For more information about convergence during solve steps, use the command:

```
pdbSet Mechanics Convergence.Info <1 | 0>
```

Typical output with information level=2 is:

```
-Iter 1
lin norm 4.6088e-13 vel err 27.792
-----
      Mesh: region_1      Mater: Metal
      Org. Val. Update    New Val.   Error   Location
      Velocity_y 1.95e-05 -5.31e-05 -3.35e-05 5.20e+01 (0.00e+00 0.00e+00 4.64e-03) (UCS)
                                         (4.64e-03 0.00e+00 0.00e+00) (DFISE)
-----
      Largest update: Velocity_y in Metal @ (-3.94e-02 0.40e+00 0.00e+00) (UCS)
                                         ( 0.00e-00 0.40e+00 3.94e-02) (DFISE)
-----
Mechanics Assembly time: 0.09s
Maximum Residual 2.7020e+07 Reference Value 3.4748e+07 Tolerance 1.0000e-03
Energy 1.5095e+03 Reference Value 5.7383e+03 Tolerance 1.0000e-03
```

where:

- Org. Val. is the original value at the node.
- Update is the update at the node.
- New Val. is Org. Val. + Update.
- Maximum Residual is the maximum norm of the force residual over the entire structure.
- Energy is the square root of the maximum norm of change in energy over the entire structure.
- Location is the location (in  $\mu\text{m}$ ) of the node in both the UCS and the DF-ISE coordinate system.

---

## References

- [1] R. E. Bank *et al.*, “Transient Simulation of Silicon Devices and Circuits,” *IEEE Transactions on Electron Devices*, vol. ED-32, no. 10, pp. 1992–2007, 1985.
- [2] O. C. Zienkiewicz and R. L. Taylor, *The Finite Element Method*, Butterworth-Heinemann: Oxford, 5th ed., 2000.
- [3] K. J. Bathe and A. P. Cimento, “Some Practical Procedures for the Solution of Nonlinear Finite Element Equations,” *Computer Methods in Applied Mechanics and Engineering*, vol. 22, no. 1, pp. 59–85, 1980.

*This appendix describes the commands of Sentaurus Process.*

---

## Syntax Conventions

The commands are designed to optimize the use of the tool command language (Tcl).

The following conventions are used for the command syntax:

- Each command starts on a new line.
- A backslash (\) is used to extend a command on to multiple lines if it appears as the last character on the line. It is not included on the last line of a command. For example:

```
refinebox name= SiOxPo mask= POLY extend= 0.1 \
    extrusion.min= -1.51 extrusion.max= -1.35 min.normal.size= 0.005 \
    interface.mat.pairs= {Silicon Oxide Silicon Polysilicon}
```

- Braces – { } – indicate a list. The braces are part of the syntax.

**NOTE** Usually, Tcl lists are created using braces, but Tcl does not typically evaluate expressions enclosed by braces. However, for convenience, Sentaurus Process does evaluate all parameters that take numeric values even when enclosed by braces.

- Brackets – [ ] – indicate an optional argument. The brackets are *not* part of the syntax.
- Parentheses – ( ) – indicate grouping of arguments. The parentheses are *not* part of the syntax.
- A vertical bar – | – indicates options, only one of which can be specified. Vertical bars are *not* part of the syntax.
- Angle brackets – < > – indicate specific type of input. The angle brackets are *not* part of the syntax.

**NOTE** An exception to this is that angle brackets must be included in the syntax if units are specified in a command. For example:

```
line x location= 0<um> spacing= 0.02<um> tag= surf
```

- The following type identifiers are used:
  - <c>: Replace with a string. In general, strings are enclosed in double quotation marks (" "), for example:

```
line_edge_roughness normal= "Z" masks= {mask1} \
correlation.length= 25.00<nm> standard.deviation= 5.00<nm>
```
  - <i>: Replace with an integer.
  - <n>: Replace with a floating-point number.
  - <list>: Replace with a Tcl list of values. The list must be enclosed in braces, for example, min= {-5.0 0.0 0.0}.
  - <field>: Replace with the name of a field.
  - <material>: Replace with the name of a material.
  - <solution>: Replace with the name of a solution.
- Boolean arguments are true (or on) if they appear on the command line (for example, negative).
- Boolean arguments are false (or off) if they appear on the command line preceded by an exclamation mark (for example, !negative).

---

## Example of Command Syntax

An example of command syntax is:

```
command
    argument1=<n>[<unit1>]
    argument2=<i>
    argument3=<i>
    argument4
    ...
    ...
```

There are two types of argument:

- *Named* arguments must be specified with a value, for example, name=Germanium.
- *Unnamed* arguments supply only the value, for example, <material> would be replaced by Oxide.

If you specify units for an argument:

- Omit spaces between the value and unit.
- Include the angle brackets with the unit, for example, xlo=5<um>.

If you specify lists:

- Lists must be enclosed in braces.
- Elements in the list must be separated by space.
- You must insert space between the equal sign and the opening brace. For example:

```
transform translate= {-1 0 0}
```

---

## Common Arguments

Nearly all Sentaurus Process commands (with the exception of those implemented as Tcl procedures as well as a few others) support two common optional arguments:

- `info=<i>`

This argument sets the amount of information to be printed to the screen and the log file. It can take the value 0, 1, or 2. The default is 0, which is the minimum amount. Higher values give more details about the status of the simulation as well as model and parameter selection information. Any value greater than 2 will be interpreted as 2.

This argument can be used with any other argument combination for nearly all commands that are not Tcl procedures.

For example, to specify that more information should be printed to the screen and the log file for the `etch` command, use:

```
etch info= 2
```

- `parameters`

This argument prints all the available arguments for a command.

For example, to print the arguments for the `extract` command, use:

```
extract parameters
```

**NOTE** When you use the `parameters` argument, the complete list of arguments for that command is generated. However, some of the arguments in this list are not documented. These parameters are used for debugging purposes only.

## A: Commands

### Quantities and Units for Command Arguments

## Quantities and Units for Command Arguments

**Table 97** lists the quantities and units for arguments used in the commands. Many command arguments specify physical values. Such arguments are given a *quantity*, and any unit of a given quantity can be used. The factor listed is the value that is multiplied by the given value to convert to the default unit (which has a factor of 1).

Table 97 Quantities, units, and factors for command arguments

Quantity	Unit	Factor
Time	s	1
	ms	1.00e-03
	min	60
	hr	3600
Distance	cm	1
	Angs	1.00e-08
	nm	1.00e-07
	um	1.00e-04
	m	1.00e+02
Volume	cm <sup>3</sup>	1
	Angs <sup>3</sup>	1.00e-24
	nm <sup>3</sup>	1.00e-21
	um <sup>3</sup>	1.00e-12
	m <sup>3</sup>	1.00e+06
Dose	cm <sup>-2</sup>	1
Concentration	cm <sup>-3</sup>	1
	m <sup>-3</sup>	1.00e-06
	um <sup>-3</sup>	1.00e+12
	nm <sup>-3</sup>	1.00e+21
	Angs <sup>-3</sup>	1.00e+24

Table 97 Quantities, units, and factors for command arguments

Quantity	Unit	Factor
Velocity	cm/s	1
	Angs/hr	2.78e-12
	Angs/min	1.67e-10
	Angs/s	1.00e-08
	nm/min	1.67e-09
	nm/s	1.00e-07
	um/min	1.67e-06
Diffusivity	cm <sup>2</sup> /s	1
	um <sup>2</sup> /min	1.67e-10
Flow	l/min	1
Stress	dyn/cm <sup>2</sup>	1
	Pa	1.00e+01
	kPa	1.00e+04
	MPa	1.00e+07
	GPa	1.00e+10
	atm	1.01e+06
	torr	1.33e+03
Viscosity	poise	1
	Pa*s	1.00e+01
Energy	eV	1
	keV	1.00e+03
	MeV	1.00e+06
Temperature	C	1
	K	1
Temperature rate	C/s	1
	K/s	1
	C/min	1.67e-02
	K/min	1.67e-02
Inverted temperature	1/K	1

**A: Commands**

Quantities and Units for Command Arguments

Table 97 Quantities, units, and factors for command arguments

Quantity	Unit	Factor
Angle	degree	1
Heat flux	W/cm <sup>2</sup>	1
	nW/cm <sup>2</sup>	1.00e-09
	uW/cm <sup>2</sup>	1.00e-06
	mW/cm <sup>2</sup>	1.00e-03
Heat transfer	W/cm <sup>2</sup> /K	1
	nW/cm <sup>2</sup> /K	1.00e-09
	uW/cm <sup>2</sup> /K	1.00e-06
	mW/cm <sup>2</sup> /K	1.00e-03
Power rate	W/s	1
	W/min	1.67e-02
Force	dyn	1
	N	1.00e+05
Toughness	dyn/cm	1
	N/m	1.00e+03
Moment	dyncm	1
	Nm	1.00e+07
Mass	g	1
	amu	1.66e-24

---

## 2DOxidationSetUp

Sets the parameters for the meshing, the time-stepping, the diffusion solver, and the mechanics solver for 2D oxidation simulations.

### Syntax

```
2DOxidationSetUp
```

### Description

This command is used when 2D oxidation is required. It modifies the parameters for the meshing, the time-stepping, the diffusion solver, and the mechanics solver.

If the information (`info`) level is set to 1 or higher, this command prints the modified parameter names and their suitable range for 2D oxidation.

## A: Commands

alias

---

# alias

Sets and prints aliases.

## Syntax

```
alias <c> [<c>] [-list]
```

## Arguments

<c>

If one argument is specified, only one alias for this value is printed.

If two arguments are specified, a new alias is set.

-list

Prints a list of allowed aliases.

## Description

This interactive mode command sets and prints aliases.

If the first argument is -list, a list of allowed aliases is printed. Otherwise, only one alias corresponding to the first argument is printed.

## Examples

Set a new alias of Temperature:

```
alias Temp Temperature
```

Print the list of allowed aliases:

```
alias -list
```

Print an alias of Temp:

```
alias Temp
```

---

## ambient

Creates new ambients for material growth reactions, such as oxidation or silicidation, or creates a new epi growth mode.

### Syntax

```
ambient
  name=<c>
  (add | clear | delete | list | print)
  [epi | inert | react]
  [lkmc.atom.name=<c>] [lkmc.mass=<n>[<amu>|<g>]] [lkmc.num.atoms=<i>]
```

### Arguments

add

Creates a new ambient.

clear

Clears all known ambients (only useful in very special situations).

delete

Deletes the named ambient.

epi, inert, react

When creating a new ambient, you can set the ambient type:

- epi ambients are used to create new epi growth modes or models.
- inert ambients are used in `gas_flow` commands to create gas reactions or to dilute active ambients.
- react creates an active ambient and is used to define material growth reactions such as oxidation.

list

Returns a Tcl list of all available ambients.

`lkmc.atom.name`, `lkmc.mass`, `lkmc.num.atoms`

These arguments are needed to create ambients that can be used with the LKMC Coordinations and Coordinations.Reactions models (see [Epitaxy Models Based on Atomic Bonding on page 572](#)). The `lkmc.atom.name` argument is mandatory. These arguments set the properties of the epi gas: `lkmc.atom.name` specifies the name of the

## A: Commands

ambient

atom that the gas deposits, `lkmc.num.atoms` specifies how many atoms of the type given by `lkmc.atom.name` are in each gas molecule, and `lkmc.mass` specifies the mass of the gas molecule (*not* the atomic mass of `lkmc.atom.name`). The default unit for `lkmc.mass` is g. The default for `lkmc.num.atoms` is 1.

name

Defines the name to be used in the `diffuse`, `gas_flow`, `reaction`, and `temp_ramp` commands to identify this ambient.

print

Prints all available ambients.

### Description

The ambient names can be used in the `diffuse`, `gas_flow`, `reaction`, and `temp_ramp` commands. [Table 81 on page 647](#) lists the available ambients.

### Examples

Create a new ambient for a new oxidation model:

```
ambient name= MyO2 add react
```

Create a new ambient for a new epi growth mode or model:

```
ambient name= MyEpi add epi
```

Create the gas Silane for use with the LKMC Coordinations model exclusively (the gases Arsine, Borane, Diborane, Germane, Phosphine, Silane, and Disilane are available by default; you do not need to create them):

```
ambient name= Silane Epi add lkmc.mass= 32.1<amu> lkmc.atom.name= Silicon
```

List the available ambients:

```
ambient list
```

### See Also

[diffuse on page 935](#)

[gas\\_flow on page 964](#)

[reaction on page 1146](#)

[temp\\_ramp on page 1224](#)

---

## ArrBreak

Creates two Arrhenius expressions that depend on a break temperature.

### Syntax

```
ArrBreak <n> <n> <n> <n> <n>
```

### Arguments

<n>

The first argument is the prefactor and the second argument is the activation energy [eV] of the first Arrhenius expression.

The third argument is the prefactor and the fourth argument is the activation energy [eV] of the second Arrhenius expression.

The final argument is the break temperature [°C].

### Description

This command creates two Arrhenius expressions and switches from the first expression to the second one at the given break temperature.

The first Arrhenius expression is computed when the temperature is below the break temperature. The second Arrhenius expression is computed when the temperature is equal to or greater than the break temperature.

### Examples

Create two Arrhenius expressions –  $3.0 e^{-0.5/k_B T}$  and  $2.0 e^{-0.4/k_B T}$  – with a break temperature of 825°C. The first Arrhenius expression is computed when  $T < 825^\circ\text{C}$ , and the second Arrhenius expression is computed when  $T \geq 825^\circ\text{C}$ :

```
ArrBreak 3.0 0.5 2.0 0.4 825.0
```

**A: Commands**Arrhenius

---

# Arrhenius

Creates an Arrhenius expression.

## Syntax

```
Arrhenius <n> <n>
```

## Arguments

<n>

The first argument is the prefactor and the second argument is the activation energy [eV] of the Arrhenius expression.

## Description

This command creates an Arrhenius expression.

## Examples

Create the Arrhenius expression  $4.0 e^{-0.5/k_B T}$ :

```
Arrhenius 4.0 0.5
```

---

## beam

Creates a beam for multiple-beam etching.

### Syntax

```
beam
  name=<c>
  (direction= {<x> <y>} | incidence=<n>)
  factor=<n>
  [list]
```

### Arguments

direction

Defines the angle of incidence of the beam using a direction vector. The specified direction vector is normalized automatically to unit length.

factor

If multiple beams are defined, factor defines the relative strength of each beam.

incidence

Defines the angle of incidence of the beam. An angle of 0 is vertical. The angle is measured counterclockwise, that is, a positive angle implies a beam ray entering from the upper left towards the lower right. A negative angle implies a beam ray entering from the upper right towards the lower left.

list

Returns a Tcl list of known beams.

name

Specifies the beam name to be referenced using sources of the etch command.

### Description

This command defines the direction and relative strength of etchant beams. The beam name is referenced in the etch command. The angle of incidence of the beam can be given using direction or incidence. The relative strength factor is used to mix the strength of different beams. Etchant beams are assumed to be collimated, that is, a slight angular spread of beam direction is not taken into account.

## A: Commands

beam

### Examples

Define a vertical beam called source1 and a beam called source2 at half the strength of source1 at an angle of 10° (positive angle implies that the beam travels from the upper left to the lower right). A third beam called source3 at one-tenth the strength of source1 enters from the upper right slightly towards the lower left:

```
beam name= source1 incidence= 0 factor= 1  
beam name= source2 incidence= 10 factor= 0.5  
beam name= source3 direction= {1 -0.1} factor= 0.1
```

### See Also

[etch on page 952](#)

---

## bound

Extracts the boundary of a material or region, and returns the outline as a list of coordinates.

### Syntax

```
bound
<material> | region=<c> [list.all]
```

### Arguments

<material>

Specifying a material extracts the boundary of all regions of the specified material. See [Specifying Materials on page 18](#).

list.all

This option lists all boundary coordinates of a region with no ordering. For regions with more than one boundary, only one closed boundary will be listed by default. If this option is switched on, all boundaries will be listed in one list but with no ordering. Default: false.

region

Specifying a region extracts the boundary of that region.

### Description

This command is used to plot the limits of the regions for further processing. It returns a list of lists of coordinates of the boundary. The outer lists are distinct parts of the regions. Each outer list comprises a complete circle around that part. Each inner list contains coordinate pairs in order around the regions. The coordinate pairs are written in xy order around the material.

**NOTE** This command is not available for 3D simulations.

### Examples

Return the boundary of oxide material:

```
bound oxide
```

Return the boundary of the region named Silicon\_1:

```
bound region= Silicon_1
```

## A: Commands

boundary

---

# boundary

Controls the conversion of GC structures generated by Sentaurus Process Explorer into the boundary representation (brep) used by Sentaurus Process.

## Syntax

```
boundary
  [spx2brep.method= MLS | Standard]
  [spx2brep.mls.cellsize=<n>]
  [spx2brep.mls.decimateblockbreps]
  [spx2brep.mls.decimatebrep]
  [spx2brep.mls.prefilterdecimation]
  [spx2brep.mls.splinesmooth]
  [spx2brep.standard.decimation]
  [spx2brep.standard.decimation.accuracy=<n>]
  [spx2brep.standard.decimation.ridge.angle=<n>]
  [spx2brep.standard.decimation.shortest.edge=<n>]
  [spx2brep.standard.tolerance=<n>]
```

## Arguments

spx2brep.method

Selects the conversion method from the following options:

- MLS uses a multimaterial level set-based conversion to smooth and filter out small features in the geometry. The MLS algorithm produces guaranteed well-defined breps that are suitable for simulation, but it is considerably slower than the standard algorithm. Internally, the algorithm first performs a standard brep conversion and then filters the resulting brep using the level-set algorithm.
- Standard provides a fast conversion and, by default, it does not apply any smoothing, resulting in a *blocky* appearance of the structure. The argument spx2brep.standard.tolerance controls this conversion method. After the conversion, the brep is decimated if the spx2brep.standard.decimation option is specified.

Default: Standard.

spx2brep.mls.cellsize

Sets the resolution of the cells used by the MLS algorithm. By default, the cells are four times the size of the resolution used in the GC structure.

`spx2brep.mls.decimateblockbreps`

If specified, the MLS algorithm decomposes the domain into blocks to improve the performance of the conversion. Default: false.

`spx2brep.mls.decimatebrep`

If specified, a decimation step is performed after the brep has been processed by the MLS algorithm. Default: false.

`spx2brep.mls.prefilterdecimation`

If specified, a decimation step is performed before sending the brep to the MLS algorithm. Default: false.

`spx2brep.mls.splinesmooth`

If specified, a b-spline filter is applied to smooth the geometry during the MLS conversion. The smoothing radius is defined as  $16 \times h$ , where  $h$  is the height of the GC column. Default: true.

`spx2brep.standard.decimation`

If specified, a decimation step is performed after the GC to brep conversion. Default: true.

`spx2brep.standard.decimation.accuracy`

Sets the accuracy used during decimation. Points are removed from the brep only if the deformation induced in the structure is less than the value specified by this argument. Default value and unit:  $1.0 \times 10^{-8} \mu\text{m}$ .

`spx2brep.standard.decimation.ridge.angle`

Sets the criterion used to detect feature ridges in the structure. Feature ridges are preserved and, if possible, not deformed during the decimation process. Default value and unit:  $150^\circ$ .

`spx2brep.standard.decimation.shortest.edge`

Sets the length of the shortest edge allowed in the final brep structure. Default value and unit:  $1.0 \times 10^{-8} \mu\text{m}$ .

`spx2brep.standard.tolerance`

Specifies how much smoothing is performed on the columns during conversion. The default value is 0.0, that is, no smoothing.

The following example sets the tolerance to 5.0, which represents reasonable smoothing:

```
boundary spx2brep.standard.tolerance=5.0
```

## A: Commands

### boundary

**NOTE** Using the standard algorithm can result in nonconformal brep geometries for nonzero values of `spx2brep.standard.tolerance`. For this reason, it is recommended to set this argument only if the resulting brep structure is intended for visualization purposes.

### Description

Conversions occur when Sentaurus Process reads a TDR GC file using the `init` command. After the `init` command is executed, Sentaurus Process works as usual, using the MGOALS module to produce structures.

---

# Compatibility

Applies parameters consistent with the default values of a previous release.

## Syntax

```
Compatibility <c>
```

## Arguments

<c>

Specifies the release from which to apply parameters. Aliases are available for the release, so it is not necessary to know the release foundation letter. For example, 2016.12 can be used instead of M-2016.12.

## Description

If used, this command must be the first command in the command file, so that all subsequent commands that depend on the default values take into account the compatibility setting (see [Compatibility With Previous Releases on page 20](#)).

## Examples

Apply parameters consistent with Version M-2016.12:

```
Compatibility 2016.12
```

## A: Commands

contact

---

## contact

Defines a contact for subsequent device simulation.

**NOTE** It is recommended to define contacts at the end of the process simulation because some process steps are not implemented for structures having contacts.

**NOTE** After the contacts are inserted, the mesh may no longer be Delaunay and may cause convergence problems. In three dimensions, you can insert contacts in the boundary representation using the following to achieve a Delaunay mesh: `pdbSet Grid Contacts.In.Brep 1`. In 2D simulations, to insert contacts in the boundary representation (brep), you must also switch on the brep mode using `pdbSet Grid MGoals use.brep.2d 1`. However, you can use region-type contacts or add mesh points around the contact perimeter to obtain a Delaunay mesh in both 2D and 3D simulations.

### Syntax

```
contact
[add] [clear]
[depth=<n>] [<um>]
[left] [right] [back] [front] [top] [bottom]
[list] [list.existing] [list.region]
[merge= <list>]
[name=<c>] [new.name=<c>]
[print]
[region=<c>]
[sidewall]
[width=<n>] [<um>]
(
    [box] [<material>] [adjacent.material=<c>] [cut.mesh]
    [xlo=<n>] [<m>|<cm>|<um>|<nm>]
    [xhi=<n>] [<m>|<cm>|<um>|<nm>]
    [ylo=<n>] [<m>|<cm>|<um>|<nm>]
    [yhi=<n>] [<m>|<cm>|<um>|<nm>]
    [zlo=<n>] [<m>|<cm>|<um>|<nm>]
    [zhi=<n>] [<m>|<cm>|<um>|<nm>] |

    [point]
    [x=<n>] [<m>|<cm>|<um>|<nm>]
    [y=<n>] [<m>|<cm>|<um>|<nm>]
    [z=<n>] [<m>|<cm>|<um>|<nm>]
    [replace]
)
```

## Arguments

add

If the contact command is called multiple times with the same name, it overwrites the previous definition by default. If add is specified, the contact command will instead add to the existing contact indicated by name or create a new contact if it does not already exist.

adjacent.material

Specifies a second material for the contact. Only elements at the interface between the two materials are allowed for the contact.

box, point

Selects one of the supported contact types:

- box: Specifies a box-type contact that consists of elements at the surface of one region or material inside the box, defined for the contact. When choosing a box-type contact, the mesh is cut where the box intersects the chosen region to give an accurate size for the contact (see cut.mesh). Occasionally, this cutting produces poor quality mesh elements. In such cases, cutting can be switched off with pdbSet Grid Cut.At.Contacts 0. Use the line command to insert lines in the mesh to retain contact size accuracy if required.
- point: Specifies a region-type contact that contains all the boundary elements of one region. The region can be specified or the material and the x-, y-, and z-coordinates of one point can be specified to select the region.

**NOTE** Box-type contacts should be used to set up mechanical boundary conditions. Region-type contacts are not recommended for setting up mechanical boundary conditions.

clear

Clears the list of all contacts. If name is specified, clear removes only the specified contact.

cut.mesh

By default, when a box contact is created, the mesh is cut at the contact borders to ensure accurate contact dimensions. Specifying !cut.mesh switches off mesh cutting, providing better element quality at the contact borders, but possibly sacrificing accuracy of the contact borders. The contact will only include nodes of the existing mesh within the contact borders.

depth

Depth of the contact in micrometers.

## A: Commands

contact

left, right, back, front, top, bottom

These arguments selectively switch on certain outer boundaries where contacts will be placed. Outer boundaries are those of the simulation domain, which includes gas regions.

By default, only `top` and `bottom` are switched on, and the rest are switched off. If any of these arguments are specified, internal interfaces are switched off. In addition, `sidewall` is equivalent to specifying all these arguments.

list

Prints a list of currently defined contacts.

list.existing

Returns a list of all contacts currently existing in the bulk structure. Adding contacts to the mesh is delayed by default. However, additional contacts that do not appear in the returned list may be read directly from a file and, therefore, exist in the structure.

list.region

Prints a list of regions adjacent to the named contact.

<material>

Specifies the material for the contact. Contacts in TDR files are always defined as a set of surface elements. Only elements at the surface of volume regions of the specified material are selected. See [Specifying Materials on page 18](#).

merge

Specifies a list of contacts that must be electrically merged. If `name` is specified, a new contact with the name `name` is created, and contacts in the list are deleted.

name

Name of the contact.

new.name

Used with `name` to change the name of a contact from that specified by `name` to that specified by `new.name`.

print

Prints the contact information.

region

Name of the volume region or name of the interface region to be used for the contact. For volume regions, only surface elements of that region are selected for the contact. For interface regions, all elements of that region are selected for contacts.

replace

If specified, the material of the region of a contact is replaced by gas for point contacts in the TDR file.

**NOTE** Replacement of the contact material with gas occurs only when the TDR file is written. However, material replacement is not allowed for the boundary representation geometry that is included in the TDR file. This is needed to restart simulations from a saved TDR file. In addition, the internal structure remains unchanged while the TDR file is written. Therefore, no material replacement occurs for the internal structure.

sidewall

Allows only surface elements on the external boundary of the simulation domain (left, right, front, back) to be selected for a contact. By default, only surface elements at material interfaces and surface elements at the top and bottom of the simulation domain are selected for contacts. Default: false.

width

Width of the contact in micrometers.

x, y, z

Define the coordinates of a point for a region-type contact. If some coordinates of the point are omitted, the region is selected using the specified coordinates only. Default unit:  $\mu\text{m}$ .

xlo, xhi, ylo, yhi, zlo, zhi

Define the low and high values in each of the coordinate directions for a box-type contact. If some coordinates are omitted, the current bounds of the simulation domain are used. Default unit:  $\mu\text{m}$ .

## Description

This command defines new contacts, deletes contacts, and prints contact information. The contact command can be called multiple times with the same name if the add argument is specified. In this case, the contact will have multiple parts. Contacts are written to TDR files in the struct command. They are not otherwise used in Sentaurus Process.

## A: Commands

### contact

**NOTE** Contacts are only intended for structures written for device simulation. They must be specified immediately before the final `struct` command used to write a structure for device simulation.

**NOTE** Contacts are not transformed using the `transform` command.

**NOTE** If a TDR file containing a boundary or mesh is read into Sentaurus Process (during the `init` command), contacts defined in this file are added to the list of contacts.

## Examples

List all available contacts:

```
contact list
```

Define a contact named `gate`, which will consist of boundary elements of the region containing the point  $(-0.05, 0.0)$ . The region material will be replaced by gas:

```
contact name= gate x= -0.05 y= 0.0 replace point
```

Define a box-type contact containing the surface elements of an aluminum region inside the specified box:

```
contact box Aluminum xlo= -0.01 ylo= -0.46 xhi= 0.1 yhi= -0.16 name= source
```

Define the substrate contact at the bottom of the simulation domain, and switch off interior interfaces:

```
contact bottom name= substrate
```

Define a contact named `lfcontact` on the left side (minimum y-coordinate) and the front (maximum z-coordinate) of the simulation domain for that part of the simulation domain inside the box  $(0,0,0) \rightarrow (1,1,1)$  and not on any interior interfaces:

```
contact left front name= lfcontact xlo= 0 ylo= 0 zlo= 0 xhi= 1 yhi= 1 zhi= 1
```

Merge contacts `C1` and `C2` so that the same supply value applies to both contacts:

```
contact merge= {C1 C2}
```

## See Also

[integrate on page 1027](#)  
[line on page 1053](#)  
[struct on page 1217](#)

---

## contour

Plots a contour of the selected variable or named data field at the value specified on a 2D plot.

### Syntax

```
contour
  [color=<c>]  [name=<c>]  [print]  [value=<n>]
  [x=<n>] [<m>|<cm>|<um>|<nm>]
  [y=<n>] [<m>|<cm>|<um>|<nm>]
  [z=<n>] [<m>|<cm>|<um>|<nm>]
```

### Arguments

color

Specifies the line color of the contour. It can be any color supported by X11 hardware and named in the color database.

name

Name of the data field. It allows plots to be created without using the select command.

Default: z\_Plot\_Var.

print

Specifies that the contour values must be printed *not* plotted. The output is compatible with xgraph. In addition, a set of Tcl lists is returned.

value

Specifies the value at which the contour line should be plotted. If boron has been selected, a value of 1.0e16 would produce a line of constant boron concentration at that concentration.

x, y, z

Specify the plane on which contouring is performed. In two dimensions, they need not be specified. In three dimensions, two arguments must be specified to indicate the plane of calculation of the contour. Default unit:  $\mu\text{m}$ .

### Description

The value must be specified in the range of the computed variable. For example, if plotting log boron, the value must be in the range 10 to 20 *not* 1e10 to 1e20.

## A: Commands

### contour

The `contour` command assumes that the `plot.2d` command has been specified and that the screen is configured to plot a 2D graphic. If this has not been set, the routine most likely will produce unhelpful results.

## Examples

Draw a line at an isoconcentration of  $10^{10}$ :

```
contour value= 1e10
```

## See Also

[Compatibility on page 915](#)

[plot.2d on page 1114](#)

[slice on page 1199](#)

---

## Coordinations.Planes.Compatibility

Specifies LKMC Coordinations.Planes epitaxy growth rates using the LKMC Coordinations epitaxy model.

### Syntax

```
Coordinations.Planes.Compatibility
```

### Description

This command specifies a compatibility mode of the LKMC Coordinations model. If this model has not been switched on, this command prints a warning; otherwise, it has no effect.

If the Coordinations model has been selected, this command sets a compatibility mode such that the growth rate will be the same as that of the Coordinations.Planes model.

### Examples

```
pbSet LKMC Model Coordinations  
Coordinations.Planes.Compatibility
```

### See Also

[Planar Epitaxy Models on page 568](#)

**A: Commands**CutLine2D

---

## CutLine2D

Computes the slice angle when given a cut in wafer coordinates.

### Syntax

```
CutLine2D <x1> <y1> <x2> <y2>
```

### Arguments

<x1> <y1> <x2> <y2>

Endpoints of the simulation cutline in wafer coordinates.

### Description

Given a cut in wafer coordinates defined by the endpoints (<x1>, <y1>) and (<x2>, <y2>), the CutLine2D command computes the slice angle.

### Examples

Set the cutline for the simulation from (0,0) to (1,0):

```
init slice.angle= [CutLine2D 0 0 1.0 0]
```

### See Also

[Wafer Coordinate System on page 37](#)

[init on page 1020](#)

## define

Defines a Tcl variable.

### Syntax

```
define <name> <value>
```

### Arguments

<name>

Any user-defined parameter name.

<value>

Any number or string value.

### Description

The `define` command is equivalent to the Tcl command `set`, except that variables defined with `set` are *not* saved or re-stored in TDR files. Variables defined using the `define` command are saved or re-stored.

The `define` and `fset` commands are equivalent.

### Examples

Define the Tcl variable `LG`, which is stored in and loaded from a TDR file. It can be used in any Tcl expression:

```
define LG 0.02
```

### See Also

Tcl documentation for description of `set` syntax

## A: Commands

defineproc

---

# defineproc

Defines a Tcl procedure.

## Syntax

```
defineproc <name> { <procedure_arguments> } {  
    <body_of_procedure>  
}
```

## Arguments

<name>

Name of the Tcl procedure.

<procedure\_arguments>

Lists the arguments of the named Tcl procedure.

<body\_of\_procedure>

Describes the Tcl procedure.

## Description

The `defineproc` command is equivalent to the Tcl command `proc`, except that procedures defined with `proc` are *not* saved or re-stored in TDR files. Procedures defined using `defineproc` are saved or re-stored.

The `defineproc` and `fproc` commands are equivalent.

## Examples

Define the Tcl procedure `relerr`, which is stored in and loaded from a TDR file:

```
defineproc relerr { newVal RefVal name my_err } {  
    upvar my_err fl  
    set denom [ expr abs($newVal)+abs($RefVal)+1e-20 ]  
    set deviation [expr 100*abs(($RefVal - $newVal)/$denom)]  
    if { $deviation > 0.5 } {  
       LogFile IL0 "Compare: $name= $newVal, ref= $RefVal, relerr= $deviation  
        \n --> failed\n"  
        set fl [ expr $fl+1 ]  
    } else {  
       LogFile IL0 "Compare: $name= $newVal, ref= $RefVal, relerr= $deviation  
        ok\n"
```

```
    }  
}
```

## See Also

Tcl documentation for description of proc syntax

---

# DeleteRefinementboxes

Deletes a set of refinement boxes based on a pattern.

## Syntax

```
DeleteRefinementboxes pattern=<c>
```

## Arguments

pattern

Specifies the pattern to use.

## Description

This command finds all the refinement boxes with names that match the defined pattern and deletes them. The pattern is expanded according to standard Tcl rules.

## Examples

Delete all refinement boxes that have names such as root\_1, root\_2, and root\_3:

```
DeleteRefinementboxes pattern= "root*"
```

## A: Commands

deposit

---

# deposit

Deposits a new layer.

## Syntax

```
deposit
( [<material>] [anisotropic | crystal | fill | fourier | isotropic]
  [coord=<n>] [<m>|<cm>|<um>|<nm>]
  [thickness=<n>] [<m>|<cm>|<um>|<nm>] )
[1D] [Adaptive] [angle=<n>]
[coeffs= {<A0> <A1> <A2> ... <An>}]
[crystal.rate= {"<100>" =<n> "<110>" =<n> "<111>" =<n> "<311>" =<n>
                "<511>" =<n> "<911>" =<n> "<221>" =<n>}]
[direction= <list>]
[doping= <list>]
([<fieldname>] | [species=<c>]
  [concentration=<n>] [<m-3>|<cm-3>|<um-3>|<nm-3>])
[fields.values= <list>]
[fill.buried] [fill.buried.interface=<material>]
[fill.buried.match.surrounding]
[force.full.levelset]
[mask=<c>]
[mat.coeffs= {
  <mat1>= {<A0> <A1> <A2> ... <An>}
  <mat2>= {<A0> <A1> <A2> ... <An>}
  ...
  <matn>= {<A0> <A1> <A2> ... <An>} }]
[material=<c>]
[polygon= <list>]
[rate=<n>[<um/min>]]
[region.name=<c>]
[remesh] [repair]
[sde=<c>]
[selective.materials= <list>]
[shadowing] [shadowing.nonisotropic]
[sources= {<beam1> <beam2> ... <beamn>}]
[steps=<n>] [Strained.Lattice]
[suppress.remesh]
[temperature=<n>] [<C>|<K>]
[time=<n>] [<hr>|<min>|<s>]
[type= anisotropic | crystal | directional | fill | fourier | isotropic |
  polygon | trapezoidal]
```

## Arguments

1D

Usually, a polygon deposition automatically increases the dimension to two dimensions before performing the operation. Specify 1D to prevent this behavior.

Adaptive

If specified, Adaptive switches on adaptive meshing for deposition. Parameters for adaptive meshing are described in [Adaptive Mesh Refinement on page 729](#). The default is the return value of `pdbGet Grid Adaptive`.

angle

Specifies the sidewall angle in degrees when using `type=trapezoidal`. An angle of 90° is vertical; an angle > 90° spreads outward with increasing deposited thickness; and an angle < 90° closes inward with increasing deposited thickness. Default unit: degree.

anisotropic, crystal, fill, fourier, isotropic

Specify the type of deposition:

- `anisotropic` defaults to vertically downward deposition.
- `crystal` specifies crystal deposition.
- `fill` is used to fill the structure with the specified material up to the specified coordinate.
- `fourier` specifies Fourier-type deposition. When using Fourier deposition, the coefficients must be specified using `coeffs` or `mat.coeffs`.
- `isotropic` implies the same rate in all directions.

These deposition types must be used with `thickness` or `coord`, *not* with `rate` and `time`.

coeffs

List of single-material coefficients used in Fourier deposition.

coord

Specifies the x-coordinate for `type=fill`. Default unit:  $\mu\text{m}$ .

crystal.rate

List of deposition rates defined per crystallographic direction in the format:

```
{"<100>" =<depo_rate> "<110>" =<depo_rate> "<111>" =<depo_rate>}
```

There is no default value for any undefined rate in a given crystallographic direction.

## A: Commands

deposit

direction

Specifies the direction for directional deposition as a list of x- and y-coordinates of the deposition vector. The x-coordinate must be positive. Positive-y indicates a right-pointing deposition beam, and negative-y indicates a left-pointing beam.

doping

List of names of doping profiles that have been previously defined with the `doping` command.

<fieldname>, species, concentration

These arguments allow a doped layer to be deposited. `species` specifies the name of the data field to be incorporated (you can add a new user species this way). Instead of specifying `species`, you can specify a field name (for example, boron, arsenic, phosphorus, and indium). The default value and unit for `concentration` is  $10^{10} \text{ cm}^{-3}$ .

fields.values

List of parameters where the parameter name is the name of the field to be introduced in the deposited layer, and the value is the initial value, for example, `fields.values={Boron=1e18}`. A list of fields of any name can be initialized with this argument and, for solution variables or stress components, units are accepted.

To initialize mole fractions in alloy materials, you can either use `xMoleFraction` or `yMoleFraction` or both directly, or use the `MoleFractionFields` command (see [MoleFractionFields on page 1089](#)).

fill.buried

By default, the material is deposited on the surface exposed to the upper gas region. If the structure has buried gas bubbles, they are untouched. Use `fill.buried` to deposit the deposition material inside those gas bubbles.

fill.buried.interface

Specifies the material with which to fill gas bubbles present at a material interface.

**NOTE** The specified material must already be present in the simulation (for example, silicon).

fill.buried.match.surrounding

Similar to `fill.buried`, but instead of depositing the deposition material inside gas bubbles, this option fills gas bubbles that are completely surrounded by a single material with that material, removing the bubbles from the domain entirely. Gas bubbles at material interfaces remain unfilled but can be filled using `fill.buried.interface`.

**NOTE** This option is available only for 3D deposition.

`force.full.levelset`

By default, the simplest algorithm is chosen to perform the deposition. However, sometimes the algorithm chosen generates incorrect results if the topology of the structure is complicated. Specifying `force.full.levelset` switches on the general level-set time-stepping algorithm that correctly handles these structures.

`mask`

Name of a mask to be used for the deposition.

**NOTE** The material is deposited outside of the mask. If deposition inside the mask is required, `negative` must be specified in the `mask` command.

`mat.coeffs`

List of multimaterial coefficients  $A_0, A_1, \dots, A_n$  used in Fourier deposition with a different set of coefficients defined for each material.

`<material>`

Allows the specification of the deposited material. See [Specifying Materials on page 18](#).

`material`

Specifies the material to be deposited. Overrides the `<material>` specification.

`polygon`

Specifies a list of x- and y-coordinates for the deposition. This is used only for 2D deposition with `type=polygon`. The list of coordinates must define a single polygon with no self-intersections. The first and last points are connected implicitly to close the polygon. The specified material is deposited inside the polygon. The default unit for the coordinates is  $\mu\text{m}$ .

`rate`

Deposition rate. Default unit:  $\mu\text{m}/\text{minute}$ .

`region.name`

Name of the region created by the `deposit` command. The name must not contain an underscore (\_) or a period (.) because these characters have special meaning. The name must be different than an existing material name (see [Regionwise Parameters and Region Name-Handling on page 29](#)).

## A: Commands

deposit

remesh

Performs a remeshing after the deposition.

repair

In 3D MGOALS mode, small regions are removed automatically by default. Sometimes, this causes small gas bubbles in the structure or other problems. Use !repair to switch off the small region removal.

sde

Specifies the arguments and algorithms for 3D Sentaurus Structure Editor. By default, arguments such as rate, thickness, time, and type are translated into appropriate Sentaurus Structure Editor commands.

If an algorithm is specified, it overwrites the algorithm used by default for isotropic or anisotropic deposition, for example:

```
sde= {"algorithm" "lopx"}  
sde= {"algorithm" "lopx" "radius" 0.07}
```

selective.materials

Specifies that deposition will occur only on a list of selected materials. For 2D simulations, MGOALS is used and multiple materials can be selected. For 3D simulations, the Sentaurus Structure Editor interface is called and only one material can be selected. In either case, only one material can be deposited.

shadowing

In two dimensions, switches on the inclusion of shadowing effects if force.full.levelset is specified or for Fourier deposition. The visibility of each surface area to each beam is calculated at every level-set time step. In 3D MGOALS mode, this argument enables shadowing effects on both directional and anisotropic deposition. The interface to Sentaurus Structure Editor ignores shadowing.

shadowing.nonisotropic

Use instead of shadowing to allow the 0th-order Fourier coefficient to deposit in areas where the beam is shadowed.

sources

Defines the source beams for level-set deposition.

steps

Subdivides a deposition into more than one step. If necessary, stress relaxation is calculated at the end of each step. Default: 1.

Strained.Lattice

Specifies strained deposition.

suppress.remesh

Suppresses mesh generation and stress rebalance operations *before* 3D deposition steps. It also suppresses mesh generation and stress rebalance *after* a 3D deposition, except when initializing fields in the newly deposited layer. See [Suppressing Mesh Generation in 3D Simulations on page 793](#).

temperature

Deposition temperature used for stress relaxation only. Default value and unit: 26.85°C.

thickness

Thickness of the deposited layers. Default unit: μm.

time

Deposition time. It must be specified if the rate argument is used. Default unit: minute.

type

Explicitly specifies the type of deposition to be performed:

- type=anisotropic performs deposition in the vertical direction only, which must be used with the rate and time arguments.
- type=crystal performs crystallographic deposition. The crystal.rate argument also must be specified.
- type=directional performs anisotropic deposition using a specified direction.
- type=fill performs a fill of a specified material up to the coordinate specified with the coord argument.
- type=fourier performs Fourier deposition, which requires the coefficients to be specified with either coeffs or mat.coeffs.
- type=isotropic performs isotropic deposition, which must be used with the rate and time arguments.
- type=polygon performs a polygonal deposition (in two dimensions), which requires the polygon argument.
- type=trapezoidal performs a trapezoidal deposition, which requires the angle and thickness arguments, and using selective.materials is recommended. This is supported in 3D deposition only.

## A: Commands

deposit

### Description

This command simulates a deposition step.

### Examples

Isotropic deposition of a 0.2  $\mu\text{m}$  oxide layer:

```
deposit thickness= 0.2 oxide isotropic
```

Same as above; thickness is defined by rate and time:

```
deposit rate= {0.2} material= {oxide} type= isotropic time= 1
```

Add an intrinsic isotropic stress of  $10^9 \text{ Pa}$  to the deposited nitride layer before the post-deposition mechanics rebalancing step:

```
deposit thickness= 0.1 nitride \
fields.values= {StressELXX= 1e9<Pa> StressELYY= 1e9<Pa> \
StressELZZ= 1e9<Pa>}
```

Deposit Si<sub>0.8</sub>Ge<sub>0.2</sub>:

```
deposit thickness= 0.1<um> SiliconGermanium \
fields.values= [MoleFractionFields SiGe 0.2]
```

### See Also

[doping on page 946](#)

[mask on page 1065](#)

[mgoals on page 1083](#)

[MoleFractionFields on page 1089](#)

---

## diffuse

Simulates thermal annealing, densification, and any material growth process during annealing – oxidation, silicidation, and epitaxy.

### Syntax

```
diffuse
  (temp.ramp=<c> |
   time=<n>[<hr>|<min>|<s>] temperature=<n>[<C>|<K>])
  [Adaptive]
  [<ambient> O2 | H2O | N2O | N2 | H2 | HCl | Cl2 | Epi | LTE]
  [angles.factors= {
    [<interface_mat1>=<list>]
    [<interface_mat2>=<list>] }]
  [auto.doping= <list>]
  [coeffs= {<A0> <A1> <A2> ... <An>}]
  [crystal.rate= {"<100>"=<n> "<110>"=<n> "<111>"=<n>}]
  [delNT=<n>] [<C>|<K>]
  [delT=<n>] [<C>|<K>]
  [delTox=<n>] [<C>|<K>]
  [density.increase= <regionName>=<n> | <material>=<n>]
  [deposit.type=<c>]
  [emulated.oed]
  [emulated.oed.box=
    xmin= {<n0>[<m>|<cm>|<um>|<nm>] <n1 ... <nn> [...] }
    ymin= {<n0>[<m>|<cm>|<um>|<nm>] <n1 ... <nn> [...] }
    zmin= {<n0>[<m>|<cm>|<um>|<nm>] <n1 ... <nn> [...] }
    xmax= {<n0>[<m>|<cm>|<um>|<nm>] <n1 ... <nn> [...] }
    ymax= {<n0>[<m>|<cm>|<um>|<nm>] <n1 ... <nn> [...] }
    zmax= {<n0>[<m>|<cm>|<um>|<nm>] <n1 ... <nn> [...] } ]
  [epi.doping= <list>]
  [epi.doping.final= <list>]
  [epi.interp= linear | log]
  [epi.layers=<i>]
  [epi.model=<i>]
  [epi.resist= {[dopant1=<n>[<ohm-cm>]] [dopant2=<n>[<ohm-cm>]] ...}]
  [epi.thickness=<n>] [<m>|<cm>|<um>|<nm>]
  [eqnInfo]
  [flow<ambient>=<n>] [<l/min>]
  [flows= {
    [<ambient1>=<n>] [<l/min>]
    [<ambient2>=<n>] [<l/min>]
    ...}]
  [gas.flow=<c>]
  [iiiv.epi=<c>]
  [init=<n>] [<hr>|<min>|<s>]
```

## A: Commands

diffuse

```
[isolve] [ISSG]
[kmc] [kmc.stress] [laser] [lkmc] [lkmc.nucleate]
[mat.coeffs= {
    <mat1>= {<A0> <A1> <A2> ... <An>}
    <mat2>= {<A0> <A1> <A2> ... <An>}
    ...
    <matn>= {<A0> <A1> <A2> ... <An>} }]
[maxstep=<n>] [<hr>|<min>|<s>]
[mgoals.native]
[minT=<n>] [<C>|<K>]
[movie=<c>]
[p<ambient>=<n>] [<atm>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
[paradis.control.file=<c>] [paradis.data.file=<c>] [paradis.library=<c>]
[partial.pressure= {
    <ambient1>=<n> [<atm>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
    <ambient2>=<n> [<atm>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
    ...
}]
[pressure=<n>] [<atm>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
[ramprate=<n>] [<C/s>|<K/s>|<C/min>|<K/min>]
[reload] [reloadHeat] [reloadReact]
[repair]
[sources= {<beam1> <beam2> ... <beamn>}]
[stress.relax]
[t.final=<n>] [<C>|<K>]
[write.temp.file=<c>]
```

## Arguments

Adaptive

If specified, Adaptive switches on adaptive meshing for this diffusion step. Parameters for adaptive meshing are described in [Adaptive Meshing During Diffusion on page 737](#). The default is the return value of pdbGet Grid Adaptive.

<ambient>

Shorthand specification to set the ambient partial pressure the same as the total pressure. If an ambient is specified this way, it must be the only ambient set in the diffuse command. In addition to the oxidation-type ambients (O<sub>2</sub>, H<sub>2</sub>O, N<sub>2</sub>O, ISSG), the epitaxial ambients Epi and LTE are available.

angles.factors

Specifies interface-specific anisotropic epi growth rate factors as a numeric list. This argument specifies a piecewise linear growth rate factor versus angle for each growing interface (the factors must be between 0 and 1). For example, to create a 30° silicon facet and a 40° polysilicon facet, use:

```
angles.factors= {
```

```
EpiOnSilicon_Gas= {0.0 1.0 25.0 1.0 30 0.0}  
EpiOnPolySilicon_Gas= {0.0 1.0 35.0 1.0 40 0.0} }
```

auto.doping

List of species for which the auto-doping model will be switched on during epitaxial growth.

coeffs

List of single-material coefficients  $A_0, A_1, \dots, A_n$  used in Fourier deposition when epi.model=1 and deposit.type=fourier.

crystal.rate

List of etching rates defined per crystallographic direction in the format:

```
{"<100>"=<dep_rate> "<110>"=<dep_rate> "<111>"=<dep_rate>}
```

used for crystallographic deposition when epi.model=1 and deposit.type=crystal.

delNT

Defines the maximum temperature step during a temperature ramp-down if specified. Default unit: degree Celsius. It also can be defined globally with the command:

```
pdbSet Diffuse delNT <n>
```

delt

Defines the maximum temperature step during a temperature ramp-up if specified. Default unit: degree Celsius. It also can be defined globally with the command:

```
pdbSet Diffuse delt <n>
```

delTox

Defines the maximum temperature step during a temperature ramp for oxidation or growth if specified. Default unit: degree Celsius. It also can be defined globally with the command:

```
pdbSet Diffuse delTox <n>
```

density.increase

Density increase. The value can be specified per region <regionName>=<n> or per material <material>=<n>.

## A: Commands

diffuse

deposit.type

When epi.model=1, epitaxy is solved as a series of alternating deposition and diffuse steps. This argument specifies the deposition type. The allowed values are:

- isotropic (default)
- crystal (in which case, crystal.rate must be specified)
- fourier (in which case, either coeffs or mat.coeffs must be specified)

emulated.oed

This option switches on emulated OED during oxidation (see [Emulated Oxidation-Enhanced Diffusion on page 361](#)).

emulated.oed.box

Specifies the x-, y-, and z-coordinates of the upper-left back corners and the lower-right front corners of the cubes that enclose parts of the structure where the reaction velocity from the emulated.oed run will be applied. Default unit:  $\mu\text{m}$ .

epi.doping

List of parameters where the parameter name is the name of the species to be initialized and the value is the initial value. A list of fields of any name can be initialized with this argument and, for solution variables, units are accepted. For example:

```
epi.doping= {boron= 1e18<cm-3> GSize= 1<nm> myfield= 1}
```

For initializing alloy fields, you can use xMoleFraction, or yMoleFraction, or both of the MoleFractionFields command (see [MoleFractionFields on page 1089](#)).

epi.doping.final

List of parameters where the parameter name is the name of the species to be initialized and the value is the final value. A list of fields of any name can be initialized with this argument and, for solution variables, units are accepted. For example:

```
epi.doping.final= {boron= 1e18<cm-3> GSize= 1<nm> myfield= 1}
```

For initializing alloy fields, you can use xMoleFraction, or yMoleFraction, or both of the MoleFractionFields command (see [MoleFractionFields on page 1089](#)).

epi.interp

Specifies either a linear or logarithmic gradient of doping between the values specified by epi.doping and epi.doping.final. Default: linear.

### epi.layers

Number of layers of mesh lines required during epitaxial growth (for both `epi.model=0` and `epi.model=1`). The default is `-1`, which indicates that 10 layers should be used if `epi.model=1`, and 40 layers should be used if `epi.model=0`.

For `epi.model=0`, if the global parameter given by:

```
pdbSet Silicon Grid epi.perp.add.dist <n>
```

is set to a positive integer, `epi.layers` is ignored (whether set or not), and `epi.perp.add.dist` is used to determine the distance between mesh lines.

For `epi.model=1`, the number of layers is adjusted if the deposited layer thickness is less than the PDB parameter `Grid MinEpiDepositThickness` in SDE mode, or `Grid MinEpiDepositThicknessMGoals3D` in 3D MGOALS mode, or `LKMC Min.Epi.Deposit.Thickness` in LKMC epitaxial growth mode.

Both `epi.layers` and `epi.perp.add.dist` are used only during epitaxial growth. When remeshing occurs, the mesh for the entire structure, including the epitaxially grown region, is recreated without considering `epi.layers` and `epi.perp.add.dist`. Since remeshing can be triggered whenever the structure changes, even during epitaxial growth, you must define some refinement boxes in the epitaxially grown region to control the mesh there.

### epi.model

Specifies the epitaxial method to use:

- `epi.model=0` (default) applies a moving-boundary algorithm similar to oxidation.
- `epi.model=1` uses alternating doped deposition and inert annealing steps.

In three dimensions, `epi.model=0` is not as stable or robust as `epi.model=1`, so `epi.model=1` is recommended.

### epi.resist

List of parameters with dopant name and resistivity to calculate the background dopant concentration. If more than one dopant name appears in the list, the doping concentration is calculated individually for each dopant by ignoring the other ones.

### epi.thickness

Sets the epitaxial layer thickness to be deposited. Usually, this argument must be specified for epitaxy. However, in the case of LKMC epitaxy, which is used when `SetAtomistic` is specified, `epi.thickness` can be omitted such that growth depends solely on the growth rate parameters (see [Silicidation on page 665](#)). Default unit:  $\mu\text{m}$ .

## A: Commands

diffuse

eqnInfo

Prints the equation updates to the log file during the Newton iteration.

flow<ambient>, flows

List of gas flows in the reaction chamber. The gas flows are used to compute the partial pressures of the active ambients (those causing material growth). Flows can be specified using either a parameter name composed of flow + <ambient> (for example, flowO2 and flowHCl where O2 and HCl are ambient names) or flows that takes a list of parameters with the names of the ambients, for example:

```
flows= {O2= 1.0<l/min> HCl= 1.0<l/min>}
```

[Table 81 on page 647](#) lists the available ambients, but this list can be extended by using the ambient command. When a gas flow is specified as a combination of flows (and not when using partial pressures), a complete reaction of the ambients is assumed to occur, for example,  $O_2 + 2H_2 \rightarrow 2H_2O$ . Besides gas reactions, the addition of inert gases changes the partial pressure of the material-growing ambients. For example, if the flows of only N<sub>2</sub> and O<sub>2</sub> are specified and are equal, the partial pressure of O<sub>2</sub> will be <total pressure>/2.0 where <total pressure> is given by the pressure argument.

**NOTE** Flows and partial pressures must not be specified together in the same gas\_flow command.

gas.flow

Specifies a gas flow to be used for this diffusion step.

**NOTE** Do not use with other gas\_flow command arguments or with the temp\_ramp command.

iiiv.epi

Specifies the name of a III–V material for epitaxial growth. An ambient must not be specified if this argument is used.

init

First time step. The default is 0.0001 s, which is sometimes inappropriate for defect simulations, particularly in cases of damage. Default unit: minute.

isolve

Switches off the initial solve for models that must have an equation solved to set the initial conditions. In these cases, you can set an initial condition and switch off the default initialization.

**ISSG**

Switches on *in situ* steam-generated (ISSG) oxidation.

**kmc**

Allows the **diffuse** command to use Sentaurus Process Kinetic Monte Carlo (Sentaurus Process KMC).

**kmc.stress**

Switches on the stress effect for Sentaurus Process KMC.

**laser**

Switches on laser annealing.

**lkmc**

Invokes the lattice kinetic Monte Carlo (LKMC) model during epitaxial growth without the need to use a **SetAtomistic** simulation. The generation of the grown epitaxial surface is performed by atomistic LKMC in a way that is transparent to users. Use **lkmc** for standard continuum simulations with epitaxial LKMC growth.

**lkmc.nucleate**

Specifies whether to begin nucleation for nonselective LKMC epi for growth on oxide or nitride.

**mat.coeffs**

List of multimaterial coefficients  $A_0, A_1, \dots, A_n$  used in Fourier deposition when **epi.model=1** and **deposit.type=fourier**.

**maxstep**

Maximum time step. Default unit: minute.

**mgoals.native**

Uses MGOALS to deposit a native oxide. This is often helpful with complex structures that have several triple points.

**minT**

Minimum annealing temperature. If the diffusion temperature falls below this value, the diffusion solver is switched off. If it occurs during a ramp, the time-stepping is altered such that diffusion switches on or off exactly at this temperature. Default value and unit: 450°C .

## A: Commands

diffuse

movie

Allows you to specify actions that occur during the annealing step. For every time step of the diffusion, the string value of the movie argument is executed. It is strongly suggested not to use the movie argument to specify actions that can change meshes. For example, movie= {grid remesh} should not be used.

p<ambient>, partial.pressure

List of the partial pressures of active ambients. Partial pressure specifications must *not* be used with flow, flow<ambient>, or pressure specifications. Specify partial pressures using either a parameter name composed of p + <ambient> (for example, pO<sub>2</sub> and pN<sub>2</sub>O where O<sub>2</sub> and N<sub>2</sub>O are active ambient names) or partial.pressure that takes a list of parameters with the names of the ambients, for example:

```
partial.pressure= {O2= 1.0<atm> N2O= 1.0<atm>}
```

[Table 81 on page 647](#) lists the available ambients, but this list can be extended by using the ambient command. These partial pressures are assumed to contribute to the oxidation or user-defined reaction processes. No reaction between the species is assumed. Default unit: atm.

**NOTE** Only the partial pressures of the active ambients are used directly in the oxidation reaction equations, so setting the partial pressure of inactive (in the sense that they cause the material growth reaction) ambients such as N<sub>2</sub> or HCl has no effect.

paradis.control.file

Specifies the path to the ParaDiS control file that defines the numeric parameters for the discrete dislocation dynamics simulation (see [Sentaurus Process–ParaDiS Application Programming Interface on page 712](#)).

paradis.data.file

Specifies the path to the ParaDiS data file that defines the simulation domain and the dislocation segments.

paradis.library

Specifies the path to the directory with the ParaDiS shared library file.

pressure

The (total) pressure of the ambient gas. This setting takes effect only if flows or flow<ambient> is defined explicitly. If gas.flow is specified, the pressure is set in the corresponding gas\_flow command. Default value and unit: 1.0 atm.

`ramp_rate`

Temperature change during anneal. Default value and unit: 0.0°K/s.

`reload, reloadHeat, reloadReact`

Allows the diffusion, laser annealing, or reaction equation to be parsed at each time step.

`repair`

In 3D MGOALS mode, small regions are removed automatically by default. Sometimes, this causes small gas bubbles in the structure or other problems. Use `!repair` to switch off the removal of small regions.

`sources`

Defines deposition sources used in Fourier deposition when `epi.model=1` and `deposit.type=fourier` are specified.

`stress.relax`

Switches on relaxation of stresses during diffusion with an inert ambient. The default is true for two dimensions and false for three dimensions.

`t.final`

Final temperature for a temperature ramp-up or ramp-down. It is used if `ramp_rate` is not given. The ramp time is calculated automatically. Default unit: degree Celsius.

`temp.ramp`

Name of a temperature ramp created with the `temp_ramp` command.

`temperature`

Annealing temperature. Default unit: degree Celsius.

`time`

Annealing time. Default unit: minute.

`write.temp.file`

Stores the thermal profile created during laser annealing. The format of the file is two columns: time (in seconds) and temperature (in degree Celsius). This file can be used to create a `temp_ramp` to allow subsequent simulations to use the computed temperature profile without the need to resimulate laser annealing.

## A: Commands

diffuse

### Arguments: Deprecated

epi.dopants

List of the data fields to be incorporated into the epitaxial layer. Deprecated in favor of epi.doping.

### Description

This command performs annealing (either continuum or KMC) or, if the diffusion time is set to 0, it activates dopants and performs a stress update. The command arguments set diffusion conditions as well as time-stepping options.

Diffusion model and parameter setting are performed with the pdbSet command. The basic settings are:

```
pdbSet <material> Dopant DiffModel <model>
```

where <model> can be one of Constant, Fermi, Pair, React, ChargedFermi, ChargedPair, or ChargedReact.

Temperature ramps are specified by first creating a list of ramping steps using the temp\_ramp command. Then, the ramp is applied using temp.ramp. All temp\_ramp command arguments can be specified with the diffuse command.

To specify an oxidizing ambient, there are different methods:

- Use the shorthand <ambient> flags.
- Use flow<ambient> or p<ambient>.
- Use the gas\_flow command and set the gas.flow argument to the name set in the gas\_flow command.
- Use gas\_flow inside the temp\_ramp command, and use temp.ramp to set the name of the temp\_ramp to be used.

[Table 81 on page 647](#) lists the available ambients and includes O<sub>2</sub>, H<sub>2</sub>O, HCl, N<sub>2</sub>, H<sub>2</sub>, Cl<sub>2</sub>, and N<sub>2</sub>O, which can be used in oxidation specification, as well as two epi ambients Epi and LTE for specifying epitaxial growth. For more information on Epi and LTE, see [Epitaxy on page 267](#).

### Examples

A simple low temperature 900°C anneal for 30 s:

```
diffuse time= 30<s> temp= 900
```

An oxidation step for a thick isolation oxide:

```
diffuse time= 90 temperature= 1000 H2O
```

A diffusion step using the temperature ramp named spike:

```
diffuse temp.ramp= spike
```

### See Also

[ambient on page 905](#)  
[gas\\_flow on page 964](#)  
[temp\\_ramp on page 1224](#)  
[term on page 1232](#)

## A: Commands

doping

---

# doping

Defines a named piecewise linear doping profile that can be used with the deposit command.

## Syntax

```
doping
  field=<c> name=<c>
  (depths= <list> | times= <list>)
  stress.values= <list>
  values= <list>
  [clear] [list] [location= vertex | element] [log.grad]
```

## Arguments

clear

Clears all doping specifications.

depths, times

You can use either:

- depths to specify a numeric list of the depths at which the values are applied. Default unit:  $\mu\text{m}$ .
- times to specify a numeric list of the times at which the values are applied. This argument only works for crystallographic deposition. The unit is minutes and cannot be changed.

Only depths or times can be specified, but not both at the same time.

field

Name of the field. It can be the name of the dopant, or the mole fractions xMoleFraction or yMoleFraction. For stresses, use the field names:

- StressELXX
- StressELXY
- StressELYY
- StressELZZ
- StressELXZ
- StressELYZ

It is not necessary to specify all stress components. Those not specified are assumed to be zero initially and are updated during the stress rebalance at the end of deposition.

list

Returns the names of all doping specifications.

location

Location where the field is to be applied. Default: vertex.

log.grad

Specifies a piecewise logarithmic doping profile.

name

Name of the profile to be used in the deposit command.

stress.values

Numeric list of the values of the stress field. Default unit: dyn/cm<sup>2</sup>.

values

Numeric list of the values of the dopant field. Default unit: cm<sup>-3</sup>.

## Description

This command allows a doping profile specification that can be used inside the deposit command to add doping and other fields to the newly deposited layer (on either vertices or elements).

## Examples

Create a doping profile definition with the name init\_boron that consists of a boron profile linearly increasing from  $1\times10^{10}$  at the starting surface to  $1\times10^{20}$  at 0.1 μm and beyond in the deposited layer. This doping profile definition can be used with the deposit command to create the specified profile:

```
doping name= init_boron field= Boron values= {1e10 1e20} depths= {0 0.1}
```

Add an intrinsic isotropic stress of  $10^9$  dyn/cm<sup>2</sup> to the deposited layer before the post-deposition mechanics rebalancing step:

```
doping name= film_Sxx field= StressELXX stress.values= {1e9 1e9} depths= {0 1}
doping name= film_Syy field= StressELYY stress.values= {1e9 1e9} depths= {0 1}
doping name= film_Szz field= StressELZZ stress.values= {1e9 1e9} depths= {0 1}
```

## See Also

[deposit on page 928](#)

## A: Commands

### element

---

## element

Extracts the grid for a specified material and returns the grid as a list of coordinates.

### Syntax

```
element <material> [region]
```

### Arguments

<material>

Name of the material. See [Specifying Materials on page 18](#).

region

Limits output to only one region if specified.

### Description

This command can be used to plot the grid. It returns a list of coordinates that define the grid. Each of the outer lists makes up a continuous line through the grid. Each inner list contains coordinate pairs in order for that line.

**NOTE** This command is not available for 3D simulations.

### Examples

Return the grid of oxide material:

```
element oxide
```

---

## Enu2G

Computes the shear modulus from Young's modulus and the Poisson ratio.

### Syntax

Enu2G <n> <n>

### Arguments

<n>

The first value is Young's modulus.

The second value is the Poisson ratio.

### Description

The same units are assumed for all moduli.

### Examples

Compute the shear modulus from Young's modulus (1.620e12 dyn/cm<sup>2</sup>) and the Poisson ratio (0.28):

Enu2G 1.620e12 0.28

**A: Commands**Enu2K

---

## Enu2K

Computes the bulk modulus from Young's modulus and the Poisson ratio.

### Syntax

```
Enu2K <n> <n>
```

### Arguments

<n>

The first value is Young's modulus.

The second value is the Poisson ratio.

### Description

The same units are assumed for all moduli.

### Examples

Compute the bulk modulus from Young's modulus (1.620e12 dyn/cm<sup>2</sup>) and the Poisson ratio (0.28):

```
Enu2K 1.620e12 0.28
```

---

## equation

Allows test parsing and resolution of an equation string.

### Syntax

```
equation eqn=<c> [nodal]
```

### Arguments

eqn

String to be checked.

nodal

If specified, nodal returns the nodal part of the string specified by eqn.

### Description

The equation string is parsed, broken into pieces, and derivatives are taken and printed. This command is useful for debugging problems with the resolver and parsing, as equation strings can be tried before being run.

### Examples

Parse and resolve the string `exp(Potential*$Vti)`:

```
equation eqn= "exp(Potential*$Vti)"
```

### See Also

[solution on page 1203](#)

## A: Commands

etch

---

## etch

Removes part or all of an exposed layer.

### Syntax

```
etch
  [1D] [Adaptive] [ambient.rate=<n>] [angle=<n>]
  [angles.rates= {
    matA= {angleA0 rateA0 angleA1 rateA1 ... angleAn rateAn}
    matB= {angleB0 rateB0 angleB1 rateB1 ... angleBn rateBn}
    ...
  }]
  [anisotropic | cmp | isotropic | trapezoidal]
  [bottom.angle=<n>] [bottom.thickness=<n>]
  [coeffs= {<A0> <A1> <A2> ... <An>}]
  [coord=<n>] [<m>|<cm>|<um>|<nm>]
  [crystal.rate= {"<100>" =<n> "<110>" =<n> "<111>" =<n> "<311>" =<n>
    "<511>" =<n> "<911>" =<n> "<221>" =<n>}]
  [direction= <list>]
  [etchstop= {<mat1> <mat2> ...} [etchstop.overetch=<n>]]
  [force.full.levelset]
  [isotropic.overetch=<n>]
  [levelset.upwind]
  [mask=<c>]
  [mat.coeffs= {
    <mat1>= {<A0> <A1> <A2> ... <An>}
    <mat2>= {<A0> <A1> <A2> ... <An>}
    ...
    <matn>= {<A0> <A1> <A2> ... <An>} }]
  [<material>]
  [material= <list>]
  [polygon= <list>]
  [rate= <list>]
  [remesh] [repair] [roundness=<n>]
  [sde=<c>]
  [shadowing] [shadowing.nonisotropic]
  [sources= {<beam1> <beam2> ... <beamn>}]
  [steps=<n>]
  [suppress.remesh]
  [temperature=<n>] [<C>|<K>]
  [thickness=<n>] [<m>|<cm>|<um>|<nm>]
  [time=<n>] [<hr>|<min>|<s>]
  [type= anisotropic | cmp | cmp.flat | crystal | directional | fourier |
    isotropic | polygon | trapezoidal]
  [undercut=<n>]
```

## Arguments

1D

Usually, a polygon etching automatically increases the dimension to two dimensions before performing the operation. Set 1D to prevent this behavior.

Adaptive

If specified, Adaptive switches on adaptive meshing for this etching step. Parameters for adaptive meshing are described in [Adaptive Mesh Refinement on page 729](#). The default is the return value of `pdbGet Grid Adaptive`.

ambient.rate

Used with `type=trapezoidal` and `force.full.levelset` to approximate the underetch effect. Default unit:  $\mu\text{m}/\text{minute}$ .

angle

Specifies the etching angle for `type=trapezoidal`. Default unit: degree.

angles.rates

Specifies a set of angle rate pairs that gives a piecewise linear etch rate versus angle. To be stable, smaller angles must have a higher etch rate. Specify the etching rate to go to zero above some angle produces facets.

anisotropic, cmp, isotropic, trapezoidal

Specifies the type of etching:

- `anisotropic`: Anisotropic etching.
- `cmp`: Chemical-mechanical polishing (CMP).
- `isotropic`: Isotropic etching.
- `trapezoidal`: Trapezoidal etching.

bottom.angle

Specifies the angle for the bottom of a trapezoidal etching in three dimensions. Default unit: degree.

bottom.thickness

Specifies the thickness for the bottom of a trapezoidal etching in three dimensions. Default unit:  $\mu\text{m}$ .

## A: Commands

etch

coeffs

List of single-material coefficients  $A_0, A_1, \dots, A_n$  used in Fourier etching.

coord

The x-coordinate to work with type=cmp. Default unit:  $\mu\text{m}$ .

crystal.rate

List of etching rates defined per crystallographic direction in the format:

```
{"<100>" =<etch_rate> "<110>" =<etch_rate> "<111>" =<etch_rate>}
```

You must add a space between the double quotation mark ("") after the crystallographic direction and the equal sign. There is no default value for any undefined rate in a given crystallographic direction. Default unit:  $\mu\text{m}/\text{minute}$ .

direction

Numeric list of x-, y-, and z-values specifying the etching direction for type=directional.

**NOTE** All three values must always be specified. In two dimensions, the z-value must always be zero.

etchstop

Materials, instead of time, can be given as etch-stopping criteria. In this case, etching continues until any of the given etchstop materials is exposed. An additional overetch is performed, with a time equal to etchstop.overetch (default: 10%) multiplied by the accumulated time required to expose the first etchstop material.

In three dimensions, etchstop is ignored when Sentaurus Structure Editor is used.

**NOTE** Materials, in addition to time, can be given as etch-stopping criteria for Fourier etching. If both time and etchstop are given, Fourier etching stops when either of the two criteria is first met.

etchstop.overetch

When etchstop is defined, an additional overetch is performed when the first etchstop material becomes exposed to gas. The duration of this overetch step is the already performed etching time multiplied by etchstop.overetch. Default: 0.1 (10%).

force.full.levelset

By default, the simplest algorithm is chosen to perform the etching. However, sometimes, the algorithm chosen generates incorrect results if the topology of the structure is

complicated. Specifying `force.full.levelset` switches on the general level-set time-stepping algorithm, which correctly handles these structures.

`isotropic.overetch`

Specifies a required amount of isotropic etching following anisotropic etching. The thickness is specified as a fraction of the anisotropic component. This argument is not implemented in 3D MGOALS mode.

`levelset.upwind`

Used with `force.full.levelset` to choose the Upwind formulation of the full level-set algorithm. The Upwind algorithm is less stable and less robust than the Lax–Friedrichs algorithm, which is the default.

`mask`

Name of the mask to be used for the etching.

`mat.coeffs`

List of multimaterial coefficients  $A_0, A_1, \dots, A_n$  used in Fourier etching with a different set of coefficients defined for each material.

`<material>`

Specifies the material to be etched. See [Specifying Materials on page 18](#).

`material`

String list of materials for multimaterial etching.

`polygon`

Numeric list of x- and y-coordinates for `type=polygon`. The list of coordinates  $\{x_0\ y_0\ x_1\ y_1\ x_2\ y_2\ \dots\ x_n\ y_n\}$  defines a single polygon that must not be self-intersecting. The first and last points are connected implicitly to close the polygon. The material inside the polygon is etched. The default unit of the coordinates is  $\mu\text{m}$ .

`rate`

Numeric list of etching rates. Default unit:  $\mu\text{m}/\text{minute}$ .

`remesh`

Performs remeshing after the etching.

## A: Commands

etch

repair

In 3D MGOALS mode, small regions are removed automatically by default. Sometimes, this causes small gas bubbles in the structure or other problems. Use !repair to switch off the small region removal.

roundness

Tuning argument for the curvature of the etch sidewalls in the case of trapezoidal etching when force.full.levelset is used. The default value is 1.0. Increased values up to 2.0 or 3.0 increase the curvature of the etch sidewall calculated by the level-set solver.

sde

String used to specify parameters and algorithms for 3D Sentaurus Structure Editor. By default, arguments such as rate, thickness, time, and type are translated into appropriate Sentaurus Structure Editor commands. If an algorithm is specified using sde, it overwrites the algorithm used by default for isotropic or anisotropic etching, for example:

```
sde= {"algorithm" "lopx"}  
sde= {"algorithm" "lopx" "radius" 0.07}
```

shadowing

In two dimensions, shadowing switches on the inclusion of shadowing effects if force.full.levelset is specified or for Fourier etching. The visibility of each surface area to each beam is calculated at every level-set time step.

In 3D MGOALS mode, shadowing enables shadowing effects on both directional and anisotropic etching.

The Sentaurus Structure Editor interface ignores shadowing.

shadowing.nonisotropic

Used instead of shadowing to allow the 0th-order Fourier coefficient to etch areas where the beam is shadowed.

sources

Defines the etching source beams for level-set etching.

steps

Subdivides an etching operation into more than one step. If necessary, stress relaxation is calculated at the end of each step. Default: 1.

suppress.remesh

Suppresses mesh generation and stress rebalance operations before and after 3D etching steps (see [Suppressing Mesh Generation in 3D Simulations on page 793](#)).

temperature

Etching temperature. Default value and unit: 26.85°C.

thickness

Thickness that is removed in the etching. Default unit: μm.

time

Refers to the etching time. It must be specified if rate is used. Default value and unit: 1.0 minute.

**NOTE** If both time and etchstop are given for Fourier etching, the Fourier etching stops when either of these two criteria is met.

type

Specifies the type of etching to be performed:

- type=anisotropic performs etching in the vertical direction only and must be used with the rate and time arguments.
- type=cmp performs CMP and is used with the argument coord.
- type=cmp.flat performs CMP, except the new surface specified by coord is flattened following stress relaxation and has zero displacement.
- type=crystal performs etching in two dimensions or three dimensions using etching rates dependent on the crystallographic direction defined by the crystal.rate argument.
- type=directional performs anisotropic etching in other directions and must be used with the direction, rate, and time arguments.
- type=fourier performs angle-dependent etching in two dimensions or three dimensions where the rate-versus-angle functions are defined by a cosine series using coeffs or mat.coeffs.
- type=isotropic performs isotropic etching, which must be used with the rate and time arguments.
- type=polygon performs polygonal etching in two dimensions and is used with the polygon argument.
- type=trapezoidal performs trapezoidal etching like Taurus™ TSUPREM-4™ in two dimensions defined by the thickness, undercut, and angle arguments, and in three dimensions defined by the thickness, angle, bottom.thickness, and bottom.angle arguments.

## A: Commands

etch

undercut

Distance to etch below the nonetchable material in 2D trapezoidal etching. Default unit:  $\mu\text{m}$ .

### Description

This command etches a layer exposed to the top gas. Several materials can be etched at the same time. There are different modes to perform etching:

- The MGOALS mode uses either an analytic or a level-set method performed by the MGOALS module.
- A general level-set time-stepping mode can handle more sophisticated etching capabilities such as multimaterial etching, Fourier etching, multiple beam, and shadowing.

### Examples

Etch a  $0.2 \mu\text{m}$  silicon layer anisotropically in the direction indicated by `direction`. A mask called `m1` is used during etching:

```
etch time= 2.0 rate= {0.1} material= {silicon} type= directional \
    direction= {1.0 1.0 0.0} mask= m1
```

Etch silicon for 0.1 minute at a rate of  $1 \mu\text{m}$  per minute, using `source1` as the etching beam, including shadowing effects, and with a Fourier response to the etchant defined by  $A_0 = 0.1$  and  $A_3 = 1$ :

```
beam name= source1 factor= 1.0 incidence= -30
etch material= {silicon} shadowing sources= {source1} type= fourier \
    coeffs= {0.1 0 0 1} time= 0.1
```

Define multimaterial Fourier etching for 0.2 minutes. The Fourier coefficients for each material are given separately within `mat.coeffs`:

```
beam name= source_beam factor= 1.0 incidence= -30
etch material= {Silicon Nitride Oxide PolySi} sources= {source_beam} \
    mat.coeffs= { Silicon= {0 0.5} Nitride= {0 1} Oxide= {0 0.75} \
        PolySilicon= {0.5} } type= fourier time= 0.2
```

### See Also

[deposit on page 928](#)  
[mask on page 1065](#)  
[mgoals on page 1083](#)

## exit

Terminates the execution of Sentaurus Process.

### Syntax

```
exit
```

### Description

This command can be used in interactive mode as well as in command files.

### See Also

[fbreak on page 962](#)

[fcontinue on page 962](#)

## A: Commands

extract

---

## extract

Extracts historical data during a diffuse step.

### Syntax

```
extract
  [clear]
  [command= {<c> <c> ...}]
  [name=<c>] [print]
  [syntax.check.value=<c>]
```

### Arguments

clear

Clears the stored historical data.

command

List of commands for data interpolation.

name

Name of data extraction.

print

Returns the extracted data values as a Tcl list with all interpolated variables.

syntax.check.value

Sets a value to be returned only during syntax-checking mode. Sometimes, the value returned by a command can cause a false syntax-check error because the value returned by the command would not be the value during the normal run mode. Setting this value avoids such problems.

### Description

Specifies the commands for data extraction during a diffuse step.

The extracted historical data can be returned as a Tcl list. Typically, the extracted data is in internal units. Internal units are the centimeter-gram-second (CGS) system of units [s, cm, g, dyn/cm<sup>2</sup>, poise, cm<sup>2</sup>/s]. For example, the unit for stress is dyn/cm<sup>2</sup>.

## Examples

Extract and store the boron concentration at the position 0.04  $\mu\text{m}$  in the silicon for each diffuse step:

```
extract name= etest command= {select z= Boron interpolate Silicon x= 0.04}
```

Return the extracted data values with the extraction name `etest` in a Tcl list (for example, if two values are extracted in `etest`, the Tcl list takes the format `<time1> <value1_1> <value2_1> <time2> <value1_2> <value2_2> ...`):

```
extract print name= etest
```

Clear all stored historical data:

```
extract clear
```

## See Also

[Extracting Values During diffuse Step: extract on page 876](#)  
[interpolate on page 1033](#)

**A: Commands**

fbreak

---

## **fbreak**

Starts interactive mode.

### **Syntax**

fbreak

### **Description**

This command interrupts the execution of command files and starts the interactive mode.

### **See Also**

[exit on page 959](#)

[fcontinue](#)

---

## **fcontinue**

Resumes execution of command files.

### **Syntax**

fcontinue

### **Description**

This interactive mode command resumes the execution of command files in batch mode.

### **See Also**

[exit on page 959](#)

[fbreak](#)

## fexec

Executes system commands.

### Syntax

```
fexec
```

### Description

Executes system calls through the Tcl command `exec` (with exactly the same syntax). Using `fexec`, the system calls are not executed during syntax-checking as they would be if the plain `exec` command were used. If there is an error in the execution, this command prints an `Error in system call` message, in addition to the error output of `exec`.

### Examples

List the contents of the current directory:

```
fexec ls
```

### See Also

Tcl documentation for description of `exec` syntax

---

## fproc

The `defineproc` and `fproc` commands are equivalent.

See [defineproc on page 926](#).

---

## fset

The `define` and `fset` commands are equivalent.

See [define on page 925](#).

## A: Commands

gas\_flow

---

## gas\_flow

Specifies a gas mixture for use with the `diffuse` or `temp_ramp` command.

### Syntax

```
gas_flow
  (clear | list | name=<c> | print)
  [<ambient>]
  [flow<ambient>=<n>] [<l/min>]
  [flows= {
    [<ambient1>=<n>] [<l/min>]
    [<ambient2>=<n>] [<l/min>]
    ...}]
  [ISSG]
  [p<ambient>=<n>] [<atm>|<torr>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
  [partial.pressure= {
    [<ambient1>=<n>] [<atm>|<torr>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
    [<ambient2>=<n>] [<atm>|<torr>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
    ...}]
  [pressure=<n>] [<atm>|<torr>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
```

### Arguments

<ambient>

Shorthand specification to set the ambient partial pressure the same as the total pressure. Only active ambients can be specified in this way, and only one ambient can be specified. The active ambients are O<sub>2</sub>, H<sub>2</sub>O, and N<sub>2</sub>O.

clear

Clears the global list of gas mixtures.

flow<ambient>, flows

List of gas flows in the reaction chamber. The gas flows are used to compute the partial pressures of the active ambients (those causing material growth). You can specify flows using either a parameter name composed of `flow + <ambient>` (for example, `flowO2` and `flowHCl` where O<sub>2</sub> and HCl are ambient names) or flows that takes a list of parameters with the names of the ambients, for example:

```
flows= {O2= 1.0<l/min> HCl= 1.0<l/min>}
```

[Table 81 on page 647](#) lists the available ambients, but this list can be extended by using the `ambient` command. When a gas flow is specified as a combination of flows (and not when using partial pressures), a complete reaction of the ambients is assumed to occur, for example, O<sub>2</sub> + 2H<sub>2</sub> → 2H<sub>2</sub>O.

Besides gas reactions, the addition of inert gases changes the partial pressure of the material-growing ambients. For example, if the flows of only N<sub>2</sub> and O<sub>2</sub> are specified and are equal, the partial pressure of O<sub>2</sub> will be <total pressure>/2.0 where <total pressure> is given by pressure.

**NOTE** Flows and partial pressures must not be specified together in the same `gas_flow` command.

ISSG

Switches on *in situ* steam-generated oxidation.

list

Generates a list of gas mixtures and returns a Tcl list that can be operated on as such. The default action for commands is to print the return, so if no handling is required, this argument prints a list of names of defined gas mixtures. If a name is specified, that gas mixture only is listed with details.

name

Identifies the gas mixture description and specifies it in a `diffuse` or `temp_ramp` command.

p<ambient>, partial.pressure

List of the partial pressures of active ambients. Partial pressure specifications must *not* be used with `flows`, `flow<ambient>`, or `pressure` specifications. You can specify partial pressures using either a parameter name composed of p + <ambient> (for example, pO<sub>2</sub> and pN<sub>2</sub>O where O<sub>2</sub> and N<sub>2</sub>O are active ambient names) or `partial.pressure` that takes a list of parameters with the names of the ambients, for example:

```
partial.pressure= {O2= 1.0<atm> N2O= 1.0<atm>}
```

[Table 81 on page 647](#) lists the available ambients, but this list can be extended by using the `ambient` command. These partial pressures are assumed to contribute to the oxidation or user-defined reaction processes. No reaction between the species is assumed. Default unit: atm.

**NOTE** Only the partial pressures of the active ambients are used directly in the oxidation reaction equations, so setting the partial pressure of inactive (in the sense that they cause the material growth reaction) ambients such as N<sub>2</sub> or HCl has no effect.

pressure

The (total) pressure of the ambient gas. Default value and unit: 1.0 atm.

## A: Commands

gas\_flow

print

Prints the gas flow information.

### Description

This command specifies a gas mixture for thermal oxidation or user-defined gas material reactions, and can be set in the `diffuse` command or `temp_ramp` command. Specification in multiple `temp_ramp` commands allows changing the gas flow during a temperature ramp. If gas flows are specified by `flows`, a complete gas reaction between the contributing gas types is assumed. The partial pressure of the active ambients (for example, material-growing ambients O<sub>2</sub>, H<sub>2</sub>O, and N<sub>2</sub>O) are the quantities directly needed to compute oxidation rates.

If `flows` is specified, the partial pressures are computed from gas reactions, the mix of remaining gases after the reaction, and the total pressure. If partial pressures of the active ambients are specified, they are used directly. The default value is 0 for all arguments, except `pressure`. [Table 81 on page 647](#) lists the available ambients and includes O<sub>2</sub>, H<sub>2</sub>O, HCl, N<sub>2</sub>, H<sub>2</sub>, Cl<sub>2</sub>, and N<sub>2</sub>O as well as two epi ambients `Epi` and `LTE` that do not apply to this command.

### Examples

These are three equivalent flow specifications for the gas mixture `myflow`:

```
gas_flow name= myflow pressure= 0.8 flows= {O2= 3.1 H2O= 1.2 H2= 0.8}  
gas_flow name= myflow pressure= 0.8 flowO2= 3.1 flowH2O= 1.2 flowH2= 0.8  
gas_flow name= myflow pressure= 0.8 flowO2= 3.1 flows= {H2O= 1.2 H2= 0.8}
```

Similar syntax for partial pressures: Three equivalent specifications for the gas mixture `mypp`. When setting partial pressures, `pressure`, `flow<ambient>`, and `flows` must not be used:

```
gas_flow name= mypp partial.pressure= {O2= 3.1 H2O= 1.2}  
gas_flow name= mypp pO2= 3.1 pH2O= 1.2  
gas_flow name= mypp pO2= 3.1 partial.pressure= {H2O= 1.2}
```

### See Also

[diffuse on page 935](#)  
[term on page 1232](#)

---

## GetMoleFractionFields

Returns the fields of the constituent elements of an alloy material for a given material or region with given mole fractions.

### Syntax

```
GetMoleFractionFields <material_or_region> <alloy_material> <xMoleFraction>  
[<yMoleFraction>]
```

### Arguments

<alloy\_material>

The name of an alloy material such as SiGe or InGaAs.

<material\_or\_region>

The name of the material or region where the fields are to be added.

<xMoleFraction>, <yMoleFraction>

Sets the required mole fraction with a value between 0 and 1 inclusively. The second mole fraction <yMoleFraction> is needed when the alloy material is a quaternary material.

### Description

The constituent elements of the material (<material\_or\_region>) must be a subset of the elements of the alloy material (<alloy\_material>). Only the complementary elements of the region material are printed. In other words, only the germanium field is printed for a silicon material region for SiGe.

### Examples

Return the fields of the constituent elements of the following alloy materials:

```
sprocess> GetMoleFractionFields Si SiGe 0.3  
Germanium = 1.447530000000008e+22  
  
sprocess> GetMoleFractionFields Ge SiGe 0.3  
Silicon = 3.377569999999998e+22  
  
sprocess> GetMoleFractionFields SiGe SiGe 0.3  
Silicon = 3.377569999999998e+22 Germanium = 1.447530000000008e+22
```

**A: Commands**

## GetMoleFractionFields

Add a germanium field to the deposited silicon material with x=0.3:

```
deposit Si thickness= 0.1 fields.values= [GetMoleFractionFields Si SiGe 0.3]
```

Add a silicon field to the deposited germanium material with x=0.3:

```
deposit Ge thickness= 0.1 fields.values= [GetMoleFractionFields Ge SiGe 0.3]
```

**See Also**

[MoleFractionFields on page 1089](#)

[SetMoleFractionFields on page 1182](#)

---

## GetMoleFractionParam

Returns the expression of the interpolation of a given parameter.

### Syntax

```
GetMoleFractionParam <alloy_material> <parameter>
```

### Arguments

<alloy\_material>

The name of an alloy material such as SiGe or InGaAs.

<parameter>

Specifies a hierarchical parameter list that is identical to the parameter specification in the Parameter Database (PDB).

### Description

This command is not applicable to KMC or MC implantation parameters.

### Examples

```
sprocess> GetMoleFractionParam SiGe Int Cstar  
((( [expr [expr [Arr 1.4e27 3.18]]]))*xMoleFraction + ([expr [expr [Arr  
3.12e23 2.932]]]))*(1.0-xMoleFraction))  
  
sprocess> GetMoleFractionParam SiGe Int ChargeStates  
0 {[([expr 1.0])]} 1 {[([expr [Arr 22.5 0.25]])*xMoleFraction + ([expr [Arr  
1.68 0.0655]])*(1.0-xMoleFraction)]} -1 {[([expr [Arr 6.0 0.52]])*(1.0-  
xMoleFraction)]} 2 {[([expr [Arr 1.26e2 0.44]])*xMoleFraction]} -2 0.0  
  
sprocess> GetMoleFractionParam Ox_SiGe B Segregation  
(([expr [expr [Arr 1.0 0.0]]]))*xMoleFraction_SiliconGermanium + ([expr  
[expr [Arr 404.66 0.822]]])* (1.0-xMoleFraction_SiliconGermanium)  
  
sprocess> GetMoleFractionParam Ox_SiGe B TrappingRate_SiGe  
(([expr [expr [Arr 1.0e-14 2.0]]]))*xMoleFraction_SiliconGermanium + ([expr  
[expr [Arr 7.0e-13 2.5]]])* (1.0-xMoleFraction_SiliconGermanium)
```

---

## graphics

Controls the user interface of Sentaurus Visual (both the plot and field selection) from the command file.

### Syntax

```
graphics
[add.active] [add.dopants] [add.total] [cmd=<c>]
[display.all= <list> | all]
[display.border= <list> | all]
[display.bulk= <list> | all]
[display.field= <list> | all]
[display.mesh= <list> | all]
[field.1d.max=<n>] [field.1d.min=<n>]
[field.max= {<c>=<n> ...}] [field.min= {<c>=<n> ...}]
[field.scale= asinh | linear | log]
[fields= <list>]
[keep.aspect.ratio] [off | on]
[svisual.cmd=<c>] [update]
[xmax=<n>] [xmin=<n>] [ymax=<n>] [ymin=<n>]
```

### Arguments

add.active, add.dopants, add.total

These options are used to select the types of fields that will be displayed in one dimension and are available to be displayed in two and three dimensions. To switch off the active dopant concentrations and NetActive, use !add.active. To switch off the dopant fields, use !add.dopants. To switch off the total concentration fields, use !add.total. Default: true.

cmd

Whenever a graphics update is typically executed, a script defined by the value of cmd is executed in addition to the graphics updating.

display.all, display.border, display.bulk, display.field, display.mesh

These arguments switch on and off respective parts of a 2D or 3D structure. They all take a list of region names or material names, or all (meaning all regions or materials) as values. For each material or region in the list, that particular part of the structure will be visible. Using an exclamation mark in front of a material or region name will hide that part of the structure. In these lists, if all appears, it is processed first for convenience.

For example, to switch on the mesh in all regions of material `Silicon` and to switch off the mesh in the region named `Oxide_1`, set:

```
display.mesh= {Silicon !Oxide_1}
```

This applies similarly to `display.border`, `display.bulk`, and `display.field`. Use `display.all` to switch on or off all bulk, field, mesh, and borders simultaneously.

For example, to switch off all regions except for the material `Silicon`, use the command:

```
graphics display.bulk= {!all Silicon}
```

`field.1d.max`, `field.1d.min`

Set the data range for all fields in xy plots. These arguments specify the maximum and minimum of the y-axis of xy plots, and apply only when Sentaurus Visual displays an xy plot of field values versus depth.

For example, `field.1d.min=1e10` sets the minimum value for an xy plot.

`field.max`, `field.min`

These arguments apply only to 2D and 3D simulations when Sentaurus Visual represents field values using color contours on the structure. These arguments adjust the field values corresponding to the maximum and minimum color contours.

For example, `field.min= {Boron=1e10 Interstitial=1e7}` sets the minimum of the color range to  $10^{10} \text{ cm}^{-3}$  when boron is displayed and to  $10^7 \text{ cm}^{-3}$  when interstitial is displayed.

`field.scale`

Changes the scaling of the contours (in 2D or 3D simulations) or the y-axis of the xy plot (1D simulation). Valid values are `asinh`, `linear`, or `log`.

`fields`

Specifies which fields to display. For 1D simulations, all fields in this list are displayed on an xy plot. For 2D and 3D simulations, the first field in the list is displayed, and the remaining fields are sent to Sentaurus Visual and can be displayed using the **Data** menu (**Scalars** tab).

In addition to this list, the options `add.active`, `add.dopants`, and `add.total` control the default availability of the fields. Since these options are true by default, the active, total, and dopant fields are sent in addition to fields specified by the `fields` argument.

`keep.aspect.ratio`

Applies to 2D simulations only. The plot range can be adjusted using `xmin`, `xmax`, `ymin`, and `ymax`. By default, the aspect ratio between the x-axis and y-axis is maintained, so that

## A: Commands

### graphics

the specified plot range of those arguments is not necessarily used. To remove this restriction, specify `!keep.aspect.ratio`.

`off`, `on`

By default, graphics updating is automatically switched on when in the Sentaurus Visual interface mode (command-line option `--svi`). These options can be used as follows:

- Set `off` to switch off automatic updating of graphics.
- Set `on` to switch on automatic updating of graphics using the command given by `cmd`.

`svvisual.cmd`

Specifies a Tcl command file to be sent directly to Sentaurus Visual. Refer to the *Sentaurus™ Visual User Guide* for commands, parameters, and syntax.

`update`

Forces a graphics update. Usually this is not necessary, as the graphics are updated automatically when the structure or data changes.

`xmax`, `xmin`, `ymax`, `ymin`

These arguments set the range of the plot and can be used independently if required. The `xmin` and `xmax` arguments apply to 1D and 2D simulations. The `ymin` and `ymax` arguments apply only to 2D simulations.

By default, the aspect ratio between the x-axis and the y-axis is maintained, so the specified plot range is not necessarily used. Specify `!keep.aspect.ratio` to remove this restriction. Default unit:  $\mu\text{m}$ .

## Description

The `graphics` command controls plot settings in Sentaurus Visual and selects which fields are available for visualization. Plot settings also can be controlled directly using the user interface of Sentaurus Visual. However, if for example, the same command file is to be run and rerun, it can be very convenient to add `graphics` commands to control the plot settings instead of making adjustments repeatedly in the user interface.

The `graphics` command also can be used to display or make available nonstandard fields. By default, standard fields will be sent to Sentaurus Visual. The `fields` argument is used to extend the available list (that is, to include fields not usually stored in the TDR file).

## Examples

In one dimension, add `ITotal` to the list of fields that are displayed (or, in two dimensions and three dimensions, display `ITotal`):

```
graphics fields= {ITotal}
```

Set the minimum of the y-axis of the xy plot to  $10^{10}$ :

```
graphics field.1d.min= 1e10
```

Set the display range in two dimensions without maintaining the xy aspect ratio (the values default to the outer simulation boundaries, so only specify those boundaries to zoom in from the outer boundary):

```
graphics xmin= -0.05<um> xmax= 0.1<um> ymax= 1.0<um> !keep.aspect.ratio
```

Specify the default minimum values for various species:

```
graphics field.min= {Boron=1e15 Arsenic=1e10 Interstitial=1e7}
```

Send a special command directly to Sentaurus Visual (in this case, to adjust the plot view):

```
graphics svisual.cmd= "move_plot -position {0.09 -0.125}"
```

## See Also

*Sentaurus™ Visual User Guide*

## A: Commands

grid

---

## grid

Sets meshing parameters, performs grid operations, and computes statistics about the mesh.

### Syntax

```
grid
[Gas]
[get.bbox | get.bbox.cm | get.bbox.um | get.bulk.nodes | get.bulk.regions |
get.dimension | get.elements | get.interface.nodes |
get.interface.regions | get.max.angle | get.max.connectivity |
get.max.edge | get.max.volume | get.max.volume.ratio |
get.max.volume.ratio.location | get.min.angle | get.min.edge |
get.min.edge.vertices | get.min.volume | get.min.volume.location |
get.nodes | get.obtuse | get.total.nodes | get.total.volume | get.vertices]
[get.brep.faces | get.brep.min.angle | get.brep.min.angle.location |
get.brep.min.edge | get.brep.min.edge.location | get.brep.stats |
get.brep.vertices]
[get.interface.area] [get.mesh.stats]
[interpolate]
[<material>]
[merge]
[remesh [Adaptive] | (2D | 3D | FullD) | get.refine.check]
[rename [print.names]]
[sano.remesh] [sano.smooth]
[save.min.edge] [save.volume]
[set.Delaunay.type= boxmethod | conformal | constrained]
[set.max.connectivity=<n>]
[set.max.neighbor.ratio=<n>]
[set.max.points=<n>]
[set.min.angle=<n>]
[set.min.edge=<n> [<m> | <cm> | <um> | <nm>]]
[set.min.grid=<n> [<m> | <cm> | <um> | <nm>]]
[set.min.normal.size=<n> [<m> | <cm> | <um> | <nm>]]
[set.normal.growth.ratio.2d=<n>]
[set.normal.growth.ratio.3d=<n>]
[set.sano.list= <list>] [set.sano.materials= <list>]
[set.syntax.check.value=<c>]
[smooth.brep [
    set.delpsc.accuracy=<n> [<m> | <cm> | <um> | <nm>]
    set.delpsc.resolution=<n> [<m> | <cm> | <um> | <nm>]
    set.repair.resolution=<n> [<m> | <cm> | <um> | <nm>]]]
```

## Arguments: Regridding, Renaming, Refinement

2D, 3D, FullD

Extrudes grid to higher dimension. The `line` commands must be issued before extruding to a higher dimension. For two dimensions, at least two y-lines must have been specified. For three dimensions, two y-lines and two z-lines must have been specified. `FullD` extrudes to the highest possible dimension.

Adaptive

If specified, `Adaptive` switches on adaptive meshing if `remesh` is specified. Parameters for adaptive meshing are described in [Adaptive Mesh Refinement on page 729](#). The default is the return value of `pdbGet Grid Adaptive`.

`get.refine.check`

Returns 1 if remeshing is needed, based on refinement criteria. Otherwise, it returns 0.

`interpolate`

Performs interpolation if `remesh` is specified.

`merge`

Merges adjacent regions of the same material into one region.

**NOTE** Do not use in combination with other arguments.

`print.names`

Prints the region names if `rename` is specified.

`remesh`

If specified, the mesh is re-created using the active mesh generator.

`rename`

Renames all regions of the structure according to the material they contain and the smallest y-coordinate point of the region, that is, from the bottom of the structure upwards. Multiple regions of the same material with the smallest y-coordinate within the given coordinate interval will increase the associated index towards the positive x-axis, from left to right (see `print.names`).

`save.min.edge`

Must be used by itself. When specified, Sentaurus Process computes the smallest edge length in each direction and saves it in three fields: `MinXEdgeLength`, `MinYEdgeLength`

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### grid

(for 2D or 3D structures), and `MinZEdgeLength` (for 3D structures). In addition, this argument stores the element volumes in the field `ElementVolume`. When `set.min.edge` is specified, the average edge length in each direction is returned and can be used to set a Tcl variable, for example:

```
set aveEdgeLength [grid save.min.edge]
```

`save.volume`

Sets element volumes as element values over the mesh. This field is not updated automatically.

`set.min.grid`

Specifies the minimum-allowed grid spacing. Default unit:  $\mu\text{m}$ .

`set.syntax.check.value`

Sets a value to be returned only during syntax-checking mode. Sometimes, the value returned by a command can cause a false syntax-check error because the value returned by the command would not be the value during the normal run mode. Setting this value avoids such problems.

## Arguments: Setting Mesh Parameters

**NOTE** These arguments set the corresponding meshing parameters under `pdbSet Grid SnMesh`. See [Table 88 on page 742](#) for more details.

`set.Delaunay.type`

Sets the meshing PDB parameter `DelaunayType`. Specifies the type of mesh generated by Sentaurus Mesh. Available types are `boxmethod`, `conformal`, or `constrained`. Default: `constrained`.

`set.max.connectivity`

Sets the meshing PDB parameter `MaxConnectivity`. Specifies the maximum number of elements connected to a point in the final mesh. Default: `1e37`.

`set.max.neighbor.ratio`

Sets the meshing PDB parameter `MaxNeighborRatio`. Binary-tree smoothing is performed after refinements have been added to the binary tree. This prevents sudden changes in the element size that can be especially detrimental to mechanics results. The ratio of neighboring collinear edges in the binary tree can be adjusted with this argument. Default: `3.0`.

`set.max.points`

Sets the meshing PDB parameter `MaxPoints`. Specifies the maximum number of points allowed by the delaunization module of Sentaurus Mesh. Default: 500000.

`set.min.angle`

Sets the meshing PDB parameter `MinAngle`. Specifies the minimum angle allowed in the elements of the mesh (2D only). Default value and unit: 0°.

`set.min.edge`

Sets the meshing PDB parameter `mineedge`. Specifies the minimum edge length. Default value and unit: 2.0e-6 μm .

`set.min.normal.size`

Sets the meshing PDB parameter `min.normal.size`. Specifies the smallest normal (to the interface) mesh element size on either side of an interface. Default value and unit: 8.0e-4 μm .

`set.normal.growth.ratio.2d`

Sets the meshing PDB parameter `normal.growth.ratio.2d`. This factor is used to increase the size of the elements in the direction normal from the interface. The size of each layer equals the size of the previous layer multiplied by this factor (2D only). Default: 2.0.

`set.normal.growth.ratio.3d`

Sets the meshing PDB parameter `normal.growth.ratio.3d`. This factor is used to increase the size of the elements in the direction normal from the interface. The size of each layer equals the size of the previous layer multiplied by this factor (3D only). Default: 3.0.

## Arguments: Grid Statistics

`Gas`

By default, quality (except volume) and `bbox` measures include the gas mesh. To exclude gas in the quality or `bbox` measure, use `!Gas`.

`<material>`

If specified, limits the measured grid statistics to the specified material.

## Arguments: Reporting Grid Statistics

`get.bbox`

Prints the bounding box of the structure (coordinates in μm ).

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grid

get.bbox.cm

Prints the bounding box of the structure (coordinates in cm).

get.bbox.um

Prints the bounding box of the structure (coordinates in  $\mu\text{m}$  ).

get.bulk.nodes

Returns the number of bulk nodes.

get.bulk.regions

Returns the number of bulk regions.

get.dimension

Returns the current simulation dimension.

get.elements

Returns the number of elements.

get.interface.area

Computes the area of interfaces. It can be limited to one particular interface by specifying a material interface such as "Silicon /Oxide" ( $\mu\text{m}$  in two dimensions,  $\mu\text{m}^2$  in three dimensions).

get.interface.nodes

Returns the number of interface nodes.

get.interface.regions

Returns the number of interface regions.

get.max.angle

Returns the maximum angle in degrees between edges (two dimensions) or faces (three dimensions).

get.max.connectivity

Returns the maximum number of edges connected to a single node.

get.max.edge

Returns the maximum edge length in  $\mu\text{m}$  .

`get.max.volume`

Returns the maximum element volume ( $\mu\text{m}^2$  in two dimensions,  $\mu\text{m}^3$  in three dimensions).

`get.max.volume.ratio`

Returns the maximum ratio of volumes of two elements that share the same node (three dimensions only).

`get.max.volume.ratio.location`

Returns the location where the maximum volume ratio occurs (coordinates in  $\mu\text{m}$ ).

`get.mesh.stats`

Indicates that all bulk mesh statistics must be printed. Here, all mesh statistics are listed as command arguments if they can be individually queried. They also are printed with `get.mesh.stats` or are listed below if they are available only by using `get.mesh.stats`:

- `bbox`: Bounding box (minimum and maximum extents) of the mesh.
- `bulk.nodes`: Number of nodes in mesh excluding those in the interface meshes (this gives two nodes for each vertex on an interface and one node for each bulk vertex).
- `bulk.regions`: Number of regions in the mesh.
- `dimension`: Simulation dimension.
- `elements`: Number of elements in the mesh.
- `interface.nodes`: Number of interface nodes in mesh. This will be the same as the number of interface vertices.
- `interface.regions`: Number of interface regions in the mesh.
- `max.angle`: Maximum of all angles of all elements in the mesh.
- `max.connectivity`: Maximum number of edges sharing one vertex in the mesh.
- `max.edge`: Length of maximum edge in the mesh (in  $\mu\text{m}$ ).
- `max.volume`: Maximum element volume (in  $\mu\text{m}^D$  where D is the dimension).
- `max.volume.ratio`: Maximum ratio of volumes (larger volume to smaller volume) of neighboring elements.
- `max.volume.ratio.location`: Location where maximum ratio of volumes occurs.
- `min.angle`: Minimum of all angles of all elements in the mesh.
- `min.edge`: Length of minimum edge in the mesh (in  $\mu\text{m}$ ).

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grid

- `min.edge.vertices`: Endpoints of minimum edge.
- `min.volume`: Minimum element volume (in  $\mu\text{m}^D$  where D is the dimension).
- `min.volume.location`: Location of the center of the element with the minimum volume.
- `nodes`: Total number of nodes in mesh. At interfaces, there are three nodes for each vertex. In the bulk, there is one node for each vertex.
- `obtuse`: Percentage of triangles or tetrahedra that have obtuse angles.
- `total.nodes`: Same as `nodes`, that is, the total number of nodes in mesh.
- `total.volume`: Volume of mesh (in  $\mu\text{m}^D$  where D is the dimension).
- `vertices`: Number of vertices in mesh.

`get.min.angle`

Returns the minimum angle in degrees between edges (two dimensions) or faces (three dimensions).

`get.min.edge`

Returns the minimum edge length in  $\mu\text{m}$ .

`get.min.edge.vertices`

Returns the vertices of the minimum edge.

`get.min.volume`

Returns the element with the smallest area in two dimensions (in  $\text{cm}^2$ ) or the smallest volume in three dimensions (in  $\mu\text{m}^3$ ).

`get.min.volume.location`

Prints the location of the smallest element (coordinates in  $\mu\text{m}$ ).

`get.nodes`

Same as `get.bulk.nodes`.

`get.obtuse`

Returns the percentage of triangles or tetrahedra that have obtuse angles.

get.total.nodes

Returns the total number of nodes in the mesh. Note the difference between points and nodes: There is a node for each region sharing an interface point in addition to each point not on an interface.

get.total.volume

Returns the total volume of the bounding box (cm in one dimension, cm<sup>2</sup> in two dimensions, and cm<sup>3</sup> in three dimensions). The unit of the angles reported is degree. If none of these is chosen, all values are reported.

get.vertices

Returns the total number of vertices in the mesh.

### Arguments: Boundary Representation (Brep) Statistics Reporting

get.brep.faces

Returns the number of faces in the brep.

get.brep.min.angle

Returns the brep minimum angle in degrees.

get.brep.min.angle.location

Returns the coordinates of the minimum angle (coordinates in μm).

get.brep.min.edge

Returns the minimum edge length (in μm) (three dimensions only).

get.brep.min.edge.location

Returns the coordinates of the minimum edge length (three dimensions only) (coordinates in μm).

get.brep.stats

Indicates that all brep statistics must be printed. Here, all brep statistics are listed as command arguments if they can be individually queried. They also are printed with get.brep.stats or are listed below if they are available only by using get.brep.stats:

- brep.are.all.boundaries.on.bbox: Returns true if all outer boundaries are on a flat bounding box; otherwise, false.
- brep.bbox: Returns the bounding box of the brep.

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grid

- `brep.conformal`: Returns true if the brep is conformal; otherwise, false.
- `brep.dimension`: Returns the dimension of the brep.
- `brep.max.angle`: Returns the brep maximum angle in degrees.
- `brep.max.angle.from.flat`: Returns  $180^\circ$ -brep maximum angle (three dimensions only).
- `brep.max.angle.location`: Returns the coordinates (in  $\mu\text{m}$ ) of the maximum angle (three dimensions only).
- `brep.min.dihedral.angle`: Returns the minimum dihedral angle in degrees in the brep (three dimensions only).
- `brep.min.dihedral.angle.location`: Returns the coordinates (in  $\mu\text{m}$ ) of the minimum dihedral angle (three dimensions only).
- `brep.min.dihedral.angle.material`: Returns the material where the minimum dihedral angle is located (three dimensions only).
- `brep.regions`: Returns the number of regions in the brep.
- `brep.total.area`: Returns the total brep interface area in three dimensions or the bulk area in two dimensions (in  $\mu\text{m}^2$ ).
- `brep.total.volume`: Returns the brep volume (three dimensions only) (in  $\mu\text{m}^3$ ).

`get.brep.vertices`

Returns the number of vertices in the brep.

### Arguments: Sano Smoothing and Remeshing

`sano.remesh`

Switches on a special Sano remesh mode. Usually, remeshing based on Sano fields and Sano field creation are performed with the `UnsetAtomistic` command (see [UnsetAtomistic on page 1252](#)), which calls `grid sano.remesh` and `grid sano.smooth`. More detail is provided here if nonstandard behavior is required. During `grid sano.remesh`, certain fields – Sano fields – can be the target of adaptive refinement. By default, the list of Sano fields contain active dopants.

**NOTE** With regard to the Sano remesh mode:

- NetActive (DopingConcentration) is updated automatically using active Sano fields during sano.remesh.
- This mode does not create any new fields in the structure. Sano fields can be created using sano.smooth in a separate grid command.
- This mode does not automatically switch on adaptive meshing.

sano.smooth

Converts KMC particle distributions to finite-element fields using the Sano method. Usually this conversion is performed with the UnsetAtomistic command, which calls grid sano.remesh and grid sano.smooth (see [UnsetAtomistic on page 1252](#)). More detail is provided here if nonstandard behavior is required. The list of fields that are converted by default contains the active dopants that are present. To change this list, use set.sano.list.

**NOTE** With regard to sano.smooth:

- NetActive (DopingConcentration) is updated automatically using Sano fields during sano.smooth.
- It specifies that only KMC particles are converted to new finite-element fields on the existing mesh; no remeshing occurs.

set.sano.list

Lists the fields for sano.remesh or sano.smooth operations. By default, the list contains the active dopant concentrations. The NetActive (DopingConcentration) field is updated automatically during Sano operations and does not need to be explicitly included here.

set.sano.materials

Lists the materials where the Sano method is applied. The default is Silicon. It is not recommended to include other materials unless special care is taken to configure Sentaurus Process KMC for those materials because, by default, the KMC models are simplistic in materials other than silicon.

### Arguments: Smoothing Boundary Representation (Brep)

smooth.brep

Removes noise and sharp features by smoothing the brep. First, a multimaterial level-set (MLS) algorithm removes any noise that may be present in the brep. Second, surface remeshing creates good-quality triangles on uneven surfaces using the Delaunay

## A: Commands

### grid

refinement for piecewise smooth complex (DelPSC) algorithm. Using multithreading with the MLS algorithm is controlled by `math numThreadsMGoals`, and using multithreading with the DelPSC algorithm is controlled by `math numThreadsSnMesh`.

`set.delpsc.accuracy`

Controls the deviation between the new surface from the DelPSC algorithm and the surface from the MLS algorithm. Default unit:  $\mu\text{m}$ .

The DelPSC surface can deviate from the MLS surface by, at most, the value of `set.delpsc.accuracy`. The DelPSC vertices lie exactly on the MLS surface, but DelPSC triangles cannot lie exactly on the MLS surface *unless* the MLS surface is flat. In general, the smaller the value of `set.delpsc.accuracy` is, the smoother the DelPSC surface becomes, and the more accurate the DelPSC surface represents the MLS surface. It uses the default value from:

`pdbGet Grid Apply.Brep.DelPSC.Accuracy`

`set.delpsc.resolution`

Controls the size of small triangles in the DelPSC algorithm. Default unit:  $\mu\text{m}$ . It uses the default value from:

`pdbGet Grid Apply.Brep.DelPSC.Resolution`

`set.repair.resolution`

Specifies the level-set cell size to remove noise and sharp features by the MLS algorithm. Default unit:  $\mu\text{m}$ .

It must be, at most, one-third of the thickness of the thinnest region. Otherwise, the thin region may be considered noise and may disappear. It uses the default value from:

`pdbGet Grid Repair.Geometry.Resolution`

The amount of geometry smoothing performed by the MLS algorithm depends on both the curvatures in the input and the level-set cell size. A noisy surface has a high curvature, so it is smoothed to a large extent to remove noise. On the other hand, a planar surface has zero curvature and is well preserved. Unfortunately, a sharp corner has a theoretically infinite curvature, so it becomes a rounded corner. The specified level-set cell size is the threshold to distinguish between the noise to be removed and the features to be preserved.

## Description

This command allows you to:

- Remesh.
- Setting meshing parameters.
- Merge regions.

- Extrude.
- Rename regions.
- Measure and report on various mesh statistics.
- Measure and report on various boundary representation (referred to as *brep*) statistics.
- Convert KMC particles into finite-element fields using the Sano method.
- Remesh while adaptively refining Sano fields.

To retrieve mesh or brep statistics, you can either:

- In a single pass, all statistics can be computed and returned in a Tcl array that can be accessed by the name of the measured value, for example:

```
array set returnArray [grid get.mesh.stats]
set numNodes $returnArray(get.total.nodes)
set numElements $returnArray(get.elements)
```

- To retrieve only the required parameter, use:

```
set numNodes [grid get.nodes]
```

**NOTE** If you are interested in several mesh statistics, it is more efficient to retrieve all statistics in one pass and read them from a Tcl array.

To limit grid or brep statistics to a particular material or interface, specify the material on the command line. For example:

- To limit brep statistics to silicon, use:

```
grid get.brep.stats Silicon
```

- To limit brep statistics to the oxide–silicon interface, use:

```
grid get.brep.stats Silicon /Oxide
```

Several mesh statistics parameters compute a measure of element quality including:

- avg.element.quality (average element quality)
- best.element.quality
- worst.element.quality
- lt3.element.quality (percentage of elements whose quality is less than 0.3)
- gt6.element.quality (percentage of elements whose quality is greater than 0.6)

These arguments are computed and returned as part of `get.mesh.stats`, but they are not separately available.

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grid

**NOTE** For the purpose of this command, quality is defined as:

- Triangles:  $4.0 * \sqrt{3.0} * \text{area} / (\text{sum of side lengths})^2$ .
- Tetrahedra: The ratio of the radius of the inscribed sphere to the radius of the circumsphere.

## Examples

Recreate the mesh using currently specified refinements:

```
grid remesh
```

Report the percentage of obtuse elements in silicon:

```
grid get.obtuse silicon
```

Compute all mesh statistics, and then read the number of nodes and the number of elements from the statistics array into numNodes and numElements, respectively:

```
array set returnArray [grid get.mesh.stats]
set numNodes $returnArray(get.total.nodes)
set numElements $returnArray(get.elements)
```

To have different Sano lists for remesh versus smoothing, use the following commands:

```
KMC2PDE
grid sano.remesh set.sano.list= BActive
grid sano.smooth set.sano.list= {AsActive BActive}
pdbSet Diffuse KMC 0
pdbSet Implant MC 0
pdbSet AtomisticData 0
kmc off
```

Remove noise and sharp features from the brep:

```
grid smooth.brep set.delpsc.resolution= 0.02 set.delpsc.accuracy= 0.0002 \
      set.repair.resolution= 0.003
```

## See Also

[line on page 1053](#)

## **help**

Prints a list of all commands available in Sentaurus Process.

### **Syntax**

```
help
```

### **Description**

This command can be used in interactive mode as well as in command files.

## A: Commands

icwb

---

## icwb

IC WorkBench (ICWB)–related functions.

### Syntax

```
icwb bbox (xmin | xmax | ymin | ymax | left | right | front | back)
icwb create.all.masks
icwb dimension
icwb domain=<c>
icwb domain= [list "<domain_name1>" "<domain_name2>" ... "<domain_namen>"]
icwb filename=<c> [scale=<n>] [& !recenter]
icwb gds.file=<c> cell=<c> layer.names= {<list>} layer.numbers= {<list>}
    sim2d | sim3d= {<n>} [domain.name=<c>] [stretches= {<c>= {<n>}}]
    [scale=<n>] [& !recenter]
icwb layer.name=<c> list polygon.names
icwb list domains
icwb list (layerIDs | layerNames)
icwb list polygon.bounding.boxes layer.name=<c>
icwb list polygon.inside.points layer.name=<c>
icwb list polygon.tessellations layer.name=<c>
icwb polygon.name=<c> list.segments
icwb slice.angle.offset
icwb stretch name=<c> value=<n>
```

### Description

The keyword `icwb` introduces commands used to operate with ICWB TCAD layout files. The different uses of the keyword `icwb` are given here, along with their syntax and corresponding descriptions:

`icwb bbox (xmin | xmax | ymin | ymax | left | right | front | back)`

Returns the corresponding coordinate, which can be one of the following in either ICWB coordinates (`xmin`, `xmax`, `ymin`, `ymax`) or Sentaurus Process coordinates (`left`, `right`, `front`, `back`).

icwb create.all.masks

Faster version of the `icwb.create.all.masks` command; intended to create large masks from complex layouts.

icwb dimension

Returns the dimension of the current domain. For the following domain types, the corresponding value for `dimension` is returned:

- Point: 1
- Gauge: 2
- Highlight: 3

icwb domain=<c>  
icwb domain= [list "<domain\_name1>" "<domain\_name2>" ... "<domain\_namen>"]

Defines the current domain. Setting the name of the current domain is a prerequisite for other ICWB commands that implicitly depend on the current domain being defined.

The second variation allows for the concatenation of multiple *gauge* domains, reorientated into one linear simulation domain.

icwb filename=<c> [scale=<n>] [!recenter]

Reads an ICWB TCAD layout file with the extension `.mac`. Coordinates in the ICWB file are multiplied by the optional `scale` argument as the file is read. Translation of the ICWB file coordinates to the (0,0) origin is switched off when the `!recenter` option is specified, which is supported in 3D simulations. The ICWB TCAD layout file must be read as a prerequisite to other ICWB commands that act on the domains and masks defined in that file.

icwb gds.file=<c> cell=<c> layer.names= {<list>} layer.numbers= {<list>}  
sim2d | sim3d= {<n>} [domain.name=<c>] [stretches= {<c>= {<n>}}]  
[scale=<n>] [!recenter]

Reads a GDSII layout file:

The `gds.file` argument specifies the input GDSII file name, and `cell` specifies the cell name. You can use `?` for the cell name, in which case, the first root cell will be used. The `layer.numbers` is a list of selected layers from the cell, and `layer.names` is a list of names for those layers.

The `domain.name` argument defines the name of the simulation domain. If no name is specified, `SIM3D` is used for a 3D domain, and `SIM2D` is used for a 2D domain. The domain will be set to be the current domain automatically, so you do not need to call `icwb domain=<c>` before using other ICWB commands. However, you can call `icwb domain=<c>` to set another preferred current domain.

## A: Commands

### icwb

`sim2d | sim3d` indicates whether it is a 2D or 3D simulation domain. The simulation domain is defined by two points, with each point defined by x- and y-coordinates in the GDSII coordinate system. For two dimensions, the two points are endpoints of a segment. The segment must be horizontal or vertical in the GDSII coordinate system. For three dimensions, the two points are the two opposite corners of the simulation domain. The first point is the left-back corner and the second point is the right-front corner in the UCS.

The `stretches` argument is a list of stretches, with each stretch having a name and being defined by a segment with two points. For a 3D domain, the segment must cross the bounding box of the domain. For a 2D domain, the segment must intersect with the 2D domain.

The `scale` argument is the same as that in the `icwb filename=<c> [scale=<n>]` command. Coordinates in the GDSII file are multiplied by `scale` as the file is read in to Sentaurus Process.

Translation of the ICWB file coordinates to the (0,0) origin is switched off when the `!recenter` option is specified, which is supported in 3D simulations.

This command can be called multiple times to set multiple simulation domains. The GDSII layout file or the ICWB TCAD layout file must be read as a prerequisite to other ICWB commands that act on the domains and masks defined in that file.

`icwb layer.name=<c> list polygon.names`

Lists polygon names given a layer name.

`icwb list domains`

Queries the names of the current domains.

`icwb list (layerIDs | layerNames)`

Returns a list of layer IDs or layer names of the ICWB TCAD layout file.

`icwb list polygon.bounding.boxes layer.name=<c>`

Returns the bounding box rectangle for each polygon in the layer.

`icwb list polygon.inside.points layer.name=<c>`

Returns a point from inside each polygon in the layer.

`icwb list polygon.tessellations layer.name=<c>`

Breaks each polygon in the layer into a set of rectangles, and then returns these rectangles.

`icwb polygon.name=<c> list.segments`

Lists polygon segments given a polygon name.

`icwb slice.angle.offset`

Returns the relative angle of the active simulation domain.

`icwb stretch name=<c> value=<n>`

Applies the given stretch by the given amount to the current domains. The order of applied stretches is important since the location of other stretches can change given the application of one stretch.

**A: Commands**icwb.composite

---

## icwb.composite

Loads a GDSII file for a 2D TCAD simulation based on composite simulation domains.

### Syntax

```
icwb.composite
  cell=<c>
  composite.domain.name= {<list>}
  gds.file=<c>
  layer.names= {<list>}
  layer.numbers= {<list>}
  sim2d.list= {{<n>} {<n>}}
  [scale=<n>]
  [stretches= {<c>= {<n>}}]
```

### Arguments

cell

Specifies the cell name.

composite.domain.name

Defines the name of the composite simulation domain. The name must consist of one alphanumeric name for each 2D simulation domain. The names are combined with a plus sign. No whitespace is allowed.

gds.file

Specifies the name of the input GDSII file.

layer.names

List of the names for the layers specified using `layer.numbers`.

layer.numbers

List of the selected layers from the GDSII file specified by `gds.file`.

scale

Coordinates in the GDSII file are multiplied by the optional `scale` argument as the file is read.

sim2d.list

Defines a sequence of 2D simulation domains that are joined to form a composite 2D simulation domain.

stretches

List of stretches, with each stretch having a name and being defined by a segment with two points. For a 2D domain, the segment must intersect with the 2D domain.

## Description

This command is similar to the `icwb gds.file=<c>` command, but it applies to 2D composite simulation domains.

## Examples

The following command loads the `BCD.gds` GDSII file and activates a 2D composite simulation domain consisting of two regular simulation domains called `BJT1` and `BJT2`:

```
set LAYERS "1:0 2:0 3:0 4:0 5:0 6:0 7:0 9:0"  
set NAMES "NWELL NACTIVE PACTIVE NPLUS POLY PBASE EMIT CONT"  
icwb.composite \  
  gds.file= "BCD.gds" cell= "Inverter" scale= 1e-3 \  
  layer.numbers= $LAYERS layer.names= $NAMES \  
  composite.domain.name= "BJT1+BJT2" \  
  sim2d.list= {{6200.0 8150.0 8400.0 8150.0} {8250.0 8800.0 8250.0 9900.0}}
```

---

## icwb.contact.mask

Creates contacts for subsequent device simulations that are tied to a layer in the ICWB TCAD layout file.

### Syntax

```
icwb.contact.mask
  (label.name=<c> [distance=<n>] | layer.name=<c>)
  (box <material> [adjacent.material=<c>] [boxheight=<n>] [xhi=<n>] [xlo=<n>]
   |
   point <material> [replace] [x=<n>])
  [name=<c>] [<other_arguments>]
```

### Arguments

box, <material>, adjacent.material, boxheight, xhi, xlo

When you specify the box option, the part of the interface between the <material> and the adjacent.material that intersect the box given by the lateral extent of the layout polygon and the vertical extent given by xhi and xlo is turned into a contact.

If xlo is not specified, the vertical location of the interface is determined automatically, and the vertical extent of the box is controlled by boxheight. The default for boxheight is 0.1 μm.

label.name, distance

Name of a text label in the ICWB TCAD layout file.

Only the text label within the given distance of the active 2D simulation domain is recognized. The default for distance is 0.03 μm. Simulation domain units are used (not layout units). The distance argument has no effect for 3D simulation domains.

layer.name

Name of a layer in the ICWB TCAD layout file.

name

Name of the contact. If name is not specified, the default value is either the label name or the layer name, whichever is specified.

point, <material>, replace, x

A point-type contact contains all the boundary elements of one or more regions. The regions are identified by the specified material and the spatial coordinate of a set of one or more points.

If `layer.name` is specified, the lateral coordinates of these points are taken as a point inside each lump of the layer (if there is more than one lump).

If `label.name` is specified, the lateral coordinates are taken as the anchor points of all text labels with the given label name.

The height coordinate can be either specified explicitly with the `x` argument or computed automatically. If the `replace` option is specified, the original material of the region of the contact is replaced by gas in the TDR file.

`<other_arguments>`

Any other arguments supported by the `contact` command.

## Description

This command serves as an interface between the ICWB TCAD layout and the `contact` command by automatically obtaining the lateral placement of the contact from the specified ICWB layer or text label location, taking the vertical placement from either the `x` argument (point type) or the `xhi` and `xlo` arguments (box type) (or, if not specified, computing it internally), and passing all other options directly to the `contact` command.

The `icwb.contact.mask` command supports both box-type and point-type contacts:

- A *box-type* contact consists of elements at the surface of one region or material inside the box. The lateral extent of the box is determined automatically from the layer segment (two dimensions) or the layer polygons (three dimensions), while the vertical extent is taken from the `xlo` and `xhi` arguments of the `contact` command. If the `xlo` argument is not explicitly given, the vertical extent is determined automatically, based on the topmost interface with the material mentioned in the command call. The vertical extent of the box is controlled by `boxheight`. If a text label name is given, the layer associated with that text label is used.
- A *point-type* contact contains all the boundary elements of one region. The lateral position of the point is determined automatically as a point inside the layer segment (two dimensions) or the polygon (three dimensions), while the vertical position is taken from the `x` argument of the `contact` command. If the `x` argument is not explicitly given, the vertical position is determined automatically, based on the interfaces with the material given in the command call. If a text label name is given, the anchor point of the text label is used.

For details on how to define contacts, see [contact on page 916](#).

**NOTE** It may be advantageous to create auxiliary layers or text labels in IC WorkBench Edit/View Plus for the placement of contacts.

**NOTE** For 3D simulations, sometimes the placement of contacts in Sentaurus Process causes meshing problems. Consider using the `!cut.mesh` option of the `contact` command (see [contact on page 916](#)).

**A: Commands**  
icwb.contact.mask

## Examples

The following commands create contacts for subsequent device simulations tied to the layers named `emitter` and `pdrain`, and the text label `drain`, in the example ICWB TCAD layout file:

```
icwb.contact.mask layer.name= emitter box polysilicon \
    adjacent.material= oxide xlo= -2.05 xhi= -1.95
icwb.contact.mask layer.name= pdrain name= drain point aluminum replace \
    x= -2.0
icwb.contact.mask label.name= "drain" point Aluminum replace
```

---

## icwb.create.all.masks

Creates positive and negative mask versions for all layers found in the currently active ICWB simulation domain.

### Syntax

```
icwb.create.all.masks
[save.to.tdr= 0 | 1]
[shift= {<dy> <dz>}]
[stretchypos= {<yo> <dy>}] [stretchyneg= {<yo> <dy>}]
[stretchzpos= {<zo> <dz>}] [stretchzneg= {<zo> <dz>}]
[reflecty= <yo>] [reflectz= <zo>]
```

### Arguments

See [icwb.create.mask on page 998](#).

### Description

The names of the masks are given by the layer names and the suffix `_p` for the positive and `_n` for the negative version of the mask.

For example, if the TCAD layout contains a layer with the name TRENCH, the corresponding mask names are `TRENCH_p` and `TRENCH_n`.

This command makes two calls to the `icwb.create.mask` command for each layer it finds in the layout file. Therefore, this command supports the `reflect*`, `save.to.tdr`, `shift`, and `stretch*` arguments of the `icwb.create.mask` command.

**NOTE** Use the command-line option `-n` to suppress automatic syntax-checking in Sentaurus Process when using this feature. The syntax-checker cannot determine which masks are available. Therefore, it may incorrectly flag the use of an unknown mask.

---

## icwb.create.mask

Creates a mask for subsequent use in `etch`, `deposit`, or `photo` commands from one or more ICWB layers.

### Syntax

```
icwb.create.mask
layer.name= <c> | <list>
[name=<c>] [polarity= positive | negative]
[save.to.tdr= 0 | 1]
[shift= {<dy> <dz>}]
[stretchypos= {<yo> <dy>}] [stretchyneg= {<yo> <dy>}]
[stretchzpos= {<zo> <dz>}] [stretchzneg= {<zo> <dz>}]
[reflecty= <yo>] [reflectz= <zo>]
```

### Arguments

`layer.name`

Name of one or more layers in the ICWB TCAD layout file. If more than one layer name is given, the resulting mask is the union of the polygons (3D) or segments (2D) from all the layers listed. (Use the `icwb list layerNames` command to obtain a list of all layer names.)

`name`

Name of the mask. The mask name defaults to the layer name. If the layer name list contains more than one entry, the first layer name is used.

`polarity`

Sets the polarity. Select `negative` to invert a mask. The polarity is assumed to be `positive` by default, that is, points inside the mask are considered masked.

`reflecty`

Reflects the layer around the y-axis defined by the given coordinate before creating the mask.

`reflectz`

Reflects the layer around the z-axis defined by the given coordinate before creating the mask.

save.to.tdr

If `save.to.tdr=0`, the created masks are not saved in a TDR file. If `save.to.tdr=1`, the mask is saved in a TDR file if – *and only if* – the total number points in the mask is less than or equal to the limit set in the PDB by the `GDS Max.Points` parameter. The default value of `save.to.tdr` is 200. If needed, you can increase this limit with:

```
pdbSet GDS Max.Points <n>
```

In addition, you can suppress the saving of *any* mask created from GDSII layers by setting:

```
pdbSetBoolean GDS Save.To.TDR 0
```

shift

Shifts the layers by the specified amount before creating the mask.

stretchypos, stretchyneg, stretchzpos, stretchzneg

Stretches the layer before creating the mask. The last four characters of the arguments determine whether the stretch is applied along the y- or z-direction and whether the layer is stretched to the positive or negative side of the stretch position.

**NOTE** More than one `shift`, `stretch*`, and `reflect*` argument can be used in the `icwb.create.mask` command. As these operations may not commute, you must note the order in which these operations are applied if more than one is used. First, `shift` is applied, and then `stretchypos`, `stretchyneg`, `stretchzpos`, `stretchzneg`, `reflecty`, and finally `reflectz` are applied.

## Description

This command serves as an interface between the ICWB TCAD layout and the mask and polygon commands, and provides a convenient way to generate 1D, 2D, and 3D masks consisting of the points, segments, or polygons from one or more ICWB layers based on a dimension-independent syntax. The command automatically determines the dimension of the currently active ICWB simulation domain.

## Examples

The following commands create masks from the corresponding layers named by `layer.name`:

```
icwb.create.mask layer.name= NWELL polarity= negative  
icwb.create.mask layer.name= NWELL name= NOTNWELL  
icwb.create.mask layer.name= "NPDIFF PPDIFF NPLUG PBASE" name=STI info=1  
icwb.create.mask layer.name= 1:0 stretchyneg= {1.2 -0.25}
```

**A: Commands**

icwb.create.mask

**See Also**

[deposit on page 928](#)  
[etch on page 952](#)  
[mask on page 1065](#)  
[photo on page 1109](#)  
[polygon on page 1124](#)

---

## implant

Specifies implantation model parameters and implants an ion species into a wafer.

### Syntax

```
implant
  [angle.dependent]
  [beta=<n>] [beta2=<n>]
  [boundary.conditions= {left=<c> right=<c> front=<c> back=<c>}]
  [cap.dependent]
  [dam.suf=<c>] [dam.table=<c>] [damage] [data.suf=<c>] [dataset=<c>]
  [depth.dependent]
  [dualpearson | gaussian | pearson | pearson.s | point.response]
  [eff.caplayer.thick=<n>] [eff.channeling.suppress]
  [en.stdev=<n>] [<keV>] [energy=<n>] [<keV>]
  [file=<c>]
  [frenkel.pair.offset= {<n> <n> <n>}]
  [gamma=<n>] [gamma2=<n>]
  [ge.effect]
  [i.plus.offset= {<n> <n> <n>}]
  [imp.table=<c>]
  [lat.scale=<n>]
  [lat.scale2=<n>]
  [lat.stdev=<n>] [<m>|<cm>|<um>|<nm>]
  [lat.stdev2=<n>] [<m>|<cm>|<um>|<nm>]
  [lexp=<n>] [<um>] [lexp2=<n>] [<um>]
  [<material>]
  [min.conc=<n>] [<m-3>|<cm-3>|<um-3>|<nm-3>])
  [ratio=<n>]
  [rp=<n>] [<m>|<cm>|<um>|<nm>]
  [rp2=<n>] [<m>|<cm>|<um>|<nm>]
  [species=<c>]
  [stdev=<n>] [<m>|<cm>|<um>|<nm>]
  [stdev2=<n>] [<m>|<cm>|<um>|<nm>]
  [tables= Default | Dios | Tasch | Taurus | TSuprem4]
  [tilt=<n>] [tilt.stdev=<n>]
  [ts4.material=<c>] [ts4.prefix=<c>] [ts4.species=<c>]
  [v.plus.offset= {<n> <n> <n>}]
  [y.position=<n>] [<um>] [z.position=<n>] [<um>]

  [Adaptive] [average]
  [backscattering] [beam.dose]
  [cascades]
```

## A: Commands

### implant

```
[conformal.spec= {
    fraction=<n> |
    fraction.field=<c> |
    xdir= {x.location= {<n> <n> ...} fraction= {<n> <n> ...}}
    ydir= {x.location= {<n> <n> ...} fraction= {<n> <n> ...}}
    zdir= {x.location= {<n> <n> ...} fraction= {<n> <n> ...} }]
[contamination= {energy=<n>[<keV>] dose.fraction=<n>[<cm-2>]}]
[crit.dose=<n> [<cm-2>]
[crystaltrim | sentaurus.mc]
[data.col=<n>] [data.file=<c>]
[data.max=<n>] [data.min=<n>] [data.units=<c>]
[data.xcol=<n>] [data.xhi=<n>] [data.xlo=<n>]
[defect.model= effective.plus.n | frenkel.pair | plus.one | userdefined]
[dfactor=<n>]
[dose=<n> [<cm-2>]
[dose.rate=<n>] [<cm-2/s>]
[en.stdev=<n>]
[energy=<n>] [<eV>|<keV>|<MeV>]
[extract.moments] [extrude]
[flip ([left] | [right])]
[fp.ifactor=<n>] [fp.vfactor=<n>]
[full.molecular] [get.moments]
[iBCA] [ifactor=<n>] [ion.movie] [KMC] [load.mc]
[match= range | dose | no]
[material=<c>]
[max.iter=<n>]
[mc.dfactor=<n>] [mc.ifactor=<n>] [mc.vfactor=<n>]
[mult.rot=<i>] [mult.rot.adaptive= {<Boolean array>}] [multiply=<n>]
[oxide.thickness=<n>] [<m>|<cm>|<um>|<nm>]
[pai] [particles=<n>]
[plasma]
[plasma.deposit= {material=<c> thickness=<n> steps=<n>}]
[plasma.source= {<species1>=<n> <species2>=<n> ...}]
[point.implant]
[postprocess] [postprocessonly] [preprocess]
[primary= beam | wafer]
[profile.reshaping]
[randomize] [range.sh] [recoils]
[rotation=<n>] [<degree>]
[rp.hi=<n>] [rp.lo=<n>]
[rp2.hi=<n>] [rp2.lo=<n>] [rp.offset=<n>]
[save.implant.domain=<c>]
[secondary.ions]
[shift=<n>]
[smooth]
[smooth.distance= {<double array>}]
[smooth.field= {<list>}]
[<species>]
```

```
[temperature=<n>] [<C>|<K>]  
[tilt=<n>] [<degree>]  
[tilt.stdev=<n>]  
[tolerance=<n>]  
[ts4.backscattering]  
[vfactor=<n>]
```

## Arguments: Specifying Models and Parameters

angle.dependent

Declares the tilt- and rotation-dependent range parameters in the implantation table used. By default, the Dios tables are all set to be angle independent. For all other tables, angle-dependent moments are assumed by default.

beta

Overwrites the kurtosis found in the specified implantation table.

beta2

Overwrites the second kurtosis found in the specified implantation table for the dual-Pearson model.

boundary.conditions= {left=<c> right=<c> front=<c> back=<c>}

Specifies the unified implantation boundary conditions that will be used by both analytic and Monte Carlo implantations. Valid keywords are Periodic, Reflect, or Extend.

cap.dependent

Specifies that the implantation moments are cap (screening) layer dependent in the dual-Pearson model.

dam.suf

Specifies the file name suffix for Taurus tables that contain the required implantation damage data in the format <ion>\_damage\_in\_<material>\_<suffix>.

dam.table

Defines the implantation table containing moments for the primary and lateral damage distributions.

damage

Switches on or off the damage calculation based on the Hobler model.

## A: Commands

### implant

data.suf

Specifies the file name suffix for Taurus tables that contain the required implantation data in the format <ion>\_in\_<material>\_<suffix>.

dataset

Used for the data name that is created when an implantation is performed.

depth.dependent

Switches on or off the lateral standard-deviation depth dependency.

dualpearson, gaussian, pearson, pearson.s, point.response

Specifies which type of primary distribution function to use.

eff.caplayer.thick

Efficiency factor for the summation of layer thicknesses to calculate the total screening (cap) layer thickness. Default: 1.

eff.channeling.suppress

Switches on the effective channeling suppression model. The default is 1 for the Taurus or TSUPREM-4 mode, and 0 otherwise.

energy

Specifies the plasma implantation energy for the species. If energy is specified for a given ion species, this energy will be used for this species instead of the common energy as specified in the performing implantation branch of the implant command. Used for plasma implantation only. Default unit: keV.

en.stdev

Specifies the standard deviation of plasma implantation energy for the species. If en.stdev is specified for a given ion species, its value will be used for this species instead of the common energy as specified in the performing implantation branch of the implant command. Used for plasma implantation only. Default unit: keV.

file

Name of the file used in the point.response model and the load.mc mode.

frenkel.pair.offset

Specifies the amount of spatial shift for the frenkel.pair model. The actual shift occurs for interstitials. This argument takes a list of numeric values. The first, second, and third

values in the list are taken as the x-, y-, and z-value, respectively. The missing value is treated as zero.

gamma

Overwrites the skewness found in the specified implantation table.

gamma2

Overwrites the second skewness found in the specified implantation table for the dual-Pearson model.

ge.effect

Specifies that the effect of germanium must be taken into account if its concentration is sufficiently large. Default: false.

i.plus.offset

Specifies the amount of spatial shift for *plus* interstitials as a list of numeric values. The first, second, and third values in the list are taken as the x-, y-, and z-value, respectively. The missing value is treated as zero.

imp.table

Defines the implantation table containing moments for the primary and lateral dopant distributions.

lat.scale

Scaling factor (unitless) for the lateral standard deviation. Default: 1.

lat.scale2

Scaling factor (unitless) for the second lateral standard deviation. Default: 1.

lat.stdev

Overwrites the lateral standard deviation found in the specified implantation table. Default unit:  $\mu\text{m}$ .

lat.stdev2

Overwrites the second lateral standard deviation found in the specified implantation table for the dual-Pearson model. Default unit:  $\mu\text{m}$ .

lexp

Overwrites the linear exponential tail length found in the specified implantation table. Default unit:  $\mu\text{m}$ .

## A: Commands

implant

lexp2

Overwrites the second linear exponential tail length found in the specified implantation table. Default unit:  $\mu\text{m}$ .

<material>

Specifies a material for which specification of model parameters is performed. See [Specifying Materials on page 18](#).

min.conc

Minimum concentration of the implanted species. Default unit:  $\text{cm}^{-3}$ .

ratio

Ratio between the amorphous part of the dose and the total dose for the dual-Pearson model.

rp

Overwrites the projected range found in the specified implantation table. Default unit:  $\mu\text{m}$ .

rp2

Overwrites the second projected range found in the specified implantation table for the dual-Pearson model. Default unit:  $\mu\text{m}$ .

species

Name of one of the solution variables of the simulation, for example, Boron.

stdev

Overwrites the standard deviation found in the specified implantation table. Default unit:  $\mu\text{m}$ .

stdev2

Overwrites the second standard deviation found in the specified implantation table for the dual-Pearson model. Default unit:  $\mu\text{m}$ .

tables

Changes the implantation tables and model switches in all materials. The settings are overwritten for one particular species if species is specified. Otherwise, the implantation tables and model switches are overwritten for all species in all materials. The available options that correspond to different implantation tables are:

- Default (tables extracted from Monte Carlo simulations with Crystal-TRIM)

- `Dios` (tables used by default in Dios)
- `Tasch` (University of Texas implantation tables)
- `Taurus` (the Taurus Process tables)
- `TSuprem4` (TSUPREM-4 native implantation tables)

`tilt`

Specifies the tilt angle for the species. If `tilt` is specified for a given ion species, the tilt angle as specified is used for this species instead of the common tilt as specified in the performing implantation branch of the `implant` command. Used for plasma implantation only.

`tilt.stdev`

Specifies the standard deviation of the tilt angle for the species. If `tilt.stdev` is specified for a given ion species, its value is used for this species instead of the common value of `tilt.stdev` as specified in the performing implantation branch of the `implant` command. Used for plasma implantation only.

`ts4.material`

Specifies the name of the material as used in TSUPREM-4. This is used for TSUPREM-4-style tables only.

`ts4.prefix`

Specifies the prefix used in TSUPREM-4 native implantation tables. Valid prefixes include `default`, `none`, `ch`, `dual`, `le`, `tr`, `ut`, and `scr`.

`ts4.species`

Specifies the TSUPREM-4 implantation table name for the dopant, for example, `chboron`, `tr.arsenic`. This is used for TSUPREM-4-style tables only.

`v.plus.offset`

Specifies the amount of spatial shift for *plus* vacancies as a list of numeric values. The first, second, and third values in the list are taken as the x-, y-, and z-value, respectively. The missing value is treated as zero.

`y.position`

Point of reference in the y-direction for an automated 1D Monte Carlo run. Default unit:  $\mu\text{m}$ .

## A: Commands

### implant

`z.position`

Point of reference in the z-direction for an automated 1D Monte Carlo run. Default unit:  $\mu\text{m}$ .

## Arguments: Performing Implantation

`adaptive`

If specified, `adaptive` switches on adaptive meshing for both analytic and Monte Carlo implantation. Parameters for adaptive meshing are described in [Adaptive Meshing During Implantation on page 738](#). The default is the return value of `pdbGet Grid Adaptive`.

`average`

Specifies whether to average the as-implanted profiles over the reflected domains in the case of `TrueReflect` boundary conditions. The default is true if the tilt angle (or `tilt2D` in the case of a 2D structure) is less than  $2^\circ$ , and false otherwise.

`backscattering`

Switches on or off the integration algorithm that accounts for particles backscattered from the surface. Default: true.

`beam.dose`

Switches to beam dose control. The default is 1 for the Taurus or TSUPREM-4 mode, and 0 otherwise.

`cascades`

Runs Monte Carlo simulations in full-cascade mode. Default: false.

`conformal.spec`

Specifies a spatial-dependent conformal ratio in one of the following (mutually exclusive) ways:

- Set `fraction=<n>` to specify a uniform conformal ratio, using a value between 0 and 1.0. For example, if `fraction=0`, you will obtain standard plasma implantation results. If `fraction=1`, you will obtain fully conformal doping.
- Use the `select` command to define a scalar conformal ratio field with a value ranging from 0 to 1. This field is then specified in `fraction.field`.
- Use the piecewise linear functions `xdir`, `ydir`, and `zdir` to specify depth-dependent conformal ratios.

These functions specify conformal ratios for surface elements whose surface normals point in the x-, y-, or z-direction, respectively. If the surface normal of an element is not

aligned with either the x-, y-, or z-direction, interpolation among different directions is performed. In 2D simulations, only `xdir` and `ydir` are required. In 3D simulations, all functions are required.

The conformal ratios are specified using a pair of lists `x.location={...}` and `fraction={...}` (`x.location` and `fraction` must have the same number of elements), where `x.location` is the x-coordinate (depth).

If the depth is outside the specified range, the closest fraction will be used.

`contamination= {energy=<n> dose.fraction=<n>}`

Specifies the parameters for energy contamination implantation, where `energy` is the contaminated energy, and `dose.fraction` is the fraction of the specified dose. The contaminated dose is `dose.fraction` x `dose`, while the main implantation dose is then  $(1 - \text{dose.fraction}) \times \text{dose}$ . Default unit for `dose.fraction`:  $\text{cm}^{-2}$ .

`crit.dose`

Defines a parameter used for the point-defect profile calculation in the `plus.one` and `frenkel.pair` models in the case of analytic implantation. Default unit:  $\text{cm}^{-2}$ .

`crystaltrim, sentaurus.mc`

Selects Monte Carlo simulation of ion implantation using either Crystal-TRIM or Sentaurus MC.

`data.col`

Specifies the column number of concentration data in `data.file` used by `extract.moments`. Default: 2.

`data.file`

Specifies the file name of the data for `extract.moments`.

`data.max`

Specifies the maximum value of the concentration data to be loaded from `data.file`. Concentration data above `data.max` is ignored by `extract.moments`. Default value and unit:  $1 \times 10^{30} \text{ cm}^{-3}$ .

`data.min`

Specifies the minimum value of the concentration data to be loaded from `data.file`. Concentration data smaller than `data.min` is ignored by `extract.moments`. Default value and unit:  $1 \times 10^{14} \text{ cm}^{-3}$ .

## A: Commands

### implant

data.units

Specifies the unit of the depth (x-)coordinate in `data.file`. Valid values are um, nm, and cm. Default: um.

data.xcol

Specifies the column number of the depth (x-)coordinate in `data.file` used by `extract.moments`. Default: 1.

data.xhi

Specifies the maximum value of the depth (x-)coordinate to be loaded from `data.file`. Depths greater than `data.xhi` are ignored by `extract.moments`. Default:  $1 \times 10^{10}$ .

data.xlo

Specifies the minimum value of the depth (x-)coordinate to be loaded from `data.file`. Depths smaller than `data.xlo` are ignored by `extract.moments`. The default value is the first depth data in `data.file`.

defect.model

Selects the model used to calculate point defects:

- The `effective.plus.n` model dynamically calculates an NFactor using an energy-dependent and a dose-dependent fitting formula.
- For `frenkel.pair`, interstitial and vacancy profiles are calculated from the damage profile resulting from the last implantation.
- `plus.one` selects the '+1' model.
- The `user.defined` model allows you to define your own models.

dfactor

Scaling factor for the damage profile calculation in analytic implantation. Default: 1.

dose

Dose of the implantation. Default value and unit:  $1 \times 10^{14} \text{ cm}^{-2}$ .

dose.rate

Dose rate of the implantation. If `dose.rate` is specified in the `implant` command, its value is used with the assumption of a uniform dose rate. If it is not specified, the dose rate is calculated from the `DoseRate` Tcl procedure in `Implant.tcl`. This argument is useful for KMC simulations only.

en.stdev

Standard deviation of implantation energy for plasma implantation. Default: 0.0. Used for plasma implantation only.

energy

Implantation energy. Default value and unit: 250 keV.

extract.moments

Specifies that the `implant` command will extract the implantation moments from the ASCII data file as specified by `data.file`.

extrude

Extrudes the 1D or 2D structure into a pseudo-3D structure before analytic implantation. This makes 1D or 2D simulation results nearly identical to those in three dimensions. Default: false.

flip ([left] | [right])

Flips the profile loaded with `load.mc` to the left. Optionally, `left` and `right` are direction specifiers for the `flip` argument.

fp.ifactor

Scaling factor for the interstitial profile calculation in the `frenkel.pair` model. Used for analytic implantation only.

fp.vfactor

Scaling factor for the vacancy profile calculation in the `frenkel.pair` model. Used for analytic implantation only.

full.molecular

Follows all particles in a Crystal-TRIM or Sentaurus MC run for a molecular species. Default: true.

get.moments

Returns the implantation moments instead of performing the actual implantation. The return value of the `implant` command is a list of keyword-value pairs. For example, for the Gaussian model, the returned list would be:

```
model gaussian rp <n> stdev <n>
```

## A: Commands

implant

For the dual-Pearson model, the returned list would be:

```
model dualpearson rp <n> stdev <n> beta <n> gamma <n> rp2 <n> stdev2 <n>
beta2 <n> gamma2 <n> ratio <n>
```

Default: false.

iBCA

Switches on the improved binary collision approximation (iBCA) damage model. Used in Sentaurus MC implantations only. Default: false.

ifactor

Scaling factor for the interstitial profile calculation in the `plus.one` and `frenkel.pair` models. It is used for the `frenkel.pair` model in the case of analytic implantation only. Default: 1.

ion.movie

Plots the positions of implanted ions during a Monte Carlo run.

KMC

Switches on the KMC mode for Monte Carlo implantation. In this mode, dynamic annealing is performed using Sentaurus Process KMC.

load.mc

Loads an external profile specified with `file`. You can select either Crystal-TRIM or Sentaurus MC for an automated Monte Carlo run by setting the `model` parameter in the parameter database, for example:

```
pdbSet MCImplant model <crystaltrim | sentaurus.mc>
```

Default: `sentaurus.mc`.

match

Selects the algorithm of the simulation in multilayer structures:

- `range` (default) selects the numeric range scaling algorithm.
- `dose` selects the dose-matching algorithm.
- `no` switches off both algorithms.

material

Specifies the material for `get.moments` from which implantation moments are extracted.

Default: silicon.

`max.ITER`

Maximum number of iterations to extract the dual-Pearson implantation moments from `DATA.FILE`. Default: 500.

`MC.DFATOR`

Scaling factor for the damage profile calculated by Sentaurus MC. Default: 1.

`MC.IFATOR`

Scaling factor for the interstitial profile calculation in the `FRENKEL.PAIR` model. Used for Monte Carlo simulations only.

`MC.VFATOR`

Scaling factor for the vacancy profile calculation in the `FRENKEL.PAIR` model. Used for Monte Carlo simulations only.

`MULT.ROT`

Specifies multiple stages of implantation at different rotation angles. For example, `MULT.ROT=4` means one-quarter of the dose is implanted at the first rotation angle, the next quarter at the original rotation angle plus 90°, the next quarter at the original rotation angle plus 180°, and the last quarter at the original rotation plus 270°. Default: 1.

`MULT.ROT.ADAPTIVE`

Specifies a list of Boolean switches (1 or 0) that set the adaptive switch for each implantation rotation. The number of Booleans in the list must equal the number specified by `MULT.ROT=<i>`. If the number of Booleans specified is less than `<i>`, the remaining Booleans are assumed to be the same as the main adaptive switch. That is, if adaptive remeshing (Adaptive in the `IMPLANT` command or the PDB parameter Grid Adaptive) is true, the unspecified switches in the `MULT.ROT.ADAPTIVE` list are true as well. On the other hand, if adaptive remeshing is false, the unspecified switches in the `MULT.ROT.ADAPTIVE` list are also false.

`MULTIPLY`

Profile loaded with `LOAD.MC` is multiplied by this value.

`OXIDE.THICKNESS`

Specifies the oxide thickness for `GET.MOMENTS`. For oxide thickness-dependent implantation tables, the implantation moments are interpolated with respect to the specified oxide thickness. Default value and unit: 0.0 μm .

## A: Commands

### implant

pai

Switches on preamorphization implantation (PAI). The PAI model takes preamorphization into account by converting the damage into effective screening layer thicknesses used for the moment lookup in screening (cap) layer-dependent tables. The default is 1 for the Taurus or TSUPREM-4 mode, and 0 otherwise.

particles

Number of pseudoparticles that will start per surface segment during MC simulations.  
Default: 1000.

plasma

Switches on plasma implantation. Valid for Sentaurus MC implantations only.

plasma.deposit= {material=<c> thickness=<n> steps=<n>}

Specifies the parameters for deposition during plasma implantation, where material specifies the deposited material, thickness specifies the total thickness of the deposited material, and steps specifies the number of steps Sentaurus Process will perform alternating between Monte Carlo implantation and material deposition. The default thickness is 0.0  $\mu\text{m}$ , and the default number of steps is 1.

plasma.source= {<species1>=<n> <species2>=<n> ...}

Specifies a list of plasma ion species where <species1>, <species2>, and so on can be any predefined species, and the number after each species specifies the fraction of the total dose as specified by dose.

point.implant

Switches on the point implantation mode, in which all particles are implanted into a central location of the implanted surface. Valid for Sentaurus MC implantations only.

postprocess

Switches on postprocessing of \*\_LastImp datasets. Default: true.

postprocessonly

Postprocesses existing \*\_LastImp datasets only (implantation itself is omitted).

preprocess

Switches on preprocessing. Default: true.

**primary**

Defines the interpretation of the range and lateral range parameters:

- `beam` (default) switches to the beam projection mode. In this case, the primary moments are applied along the projection of the ion beam on to the simulation plane, and the lateral integration is performed perpendicular to the projection of the ion beam.
- `wafer` switches to the wafer normal mode. Here, the primary distribution function and the moments are interpreted orthogonally to the wafer surface.

**profile.reshaping**

Switches on the profile reshaping model. The default is 1 for the Taurus or TSUPREM-4 mode, and 0 otherwise.

**randomize**

If specified, randomizes the random seed (by using an internal clock) each time the command file is run. Therefore, each run will produce different results. Used for Monte Carlo implantations only. Default: false.

**range.sh**

Switches on the proportional range shift mode. The channeling part of the profile is shifted proportionally to the ratio of the amorphous and the channeling range. The shift is the same for both contributions if the model is switched off. The default is 1 for the Taurus or TSUPREM-4 mode, and 0 otherwise.

**recoils**

Switches to recoil implantation, for example, to simulate the oxygen knock-on effect. Used for Sentaurus MC implantations only. Default: false.

**rotation**

Rotation angle of the wafer in the implanter. Default value and unit:  $-90^\circ$ .

**rp.hi**

Specifies the maximum value for the projected range ( $r_p$ ) of the first Pearson moments extracted by `extract.moments`. Default unit:  $\mu\text{m}$ .

**rp.lo**

Specifies the minimum value for the projected range ( $r_p$ ) of the first Pearson moments extracted by `extract.moments`. Default unit:  $\mu\text{m}$ .

## A: Commands

implant

rp2.hi

Specifies the maximum value for the projected range (rp2) of the second Pearson moments extracted by extract.moments. Default unit:  $\mu\text{m}$ .

rp2.lo

Specifies the minimum value for the projected range (rp2) of the second Pearson moments extracted by extract.moments. Default unit:  $\mu\text{m}$ .

rp.offset

Specifies the offset for the projected ranges of the first and second Pearson moments extracted by extract.moments. The extracted projected ranges are shifted by rp.offset. Default value and unit: 0.0  $\mu\text{m}$ .

save.implant.domain

Specifies the name of the file that saves the reflected MC implantation domain in the boundary representation (brep) format. This argument is ignored if TrueReflect boundary conditions are not used in the MC implantation. Default: none.

secondary.ions

When this argument is switched off, secondary ion fields (for example, fluorine in a  $\text{BF}_2$  implantation) are not created for Monte Carlo implantation. Default: true.

shift

Shifts the profile loaded with load.mc by a certain amount along the y-axis. Default unit:  $\mu\text{m}$ .

smooth

Switches on smoothing of the as-implanted profiles after Monte Carlo implantation. If smooth.field is not specified, all the as-implanted profiles are smoothed. Default: false.

smooth.distance

Specifies the smoothing distance for each field as specified in smooth.field. Default value and unit: 2.0 nm.

smooth.field

Specifies a list of fields to be smoothed. The valid fields are dopant names or Damage. For example, for  $\text{BF}_2$  implantation, Boron, Fluorine, or Damage are valid names.

<species>

Any of the previously defined species names can be specified.

temperature

Implantation temperature (wafer temperature). Default value and unit: 26.84°C .

tilt

Angle normal to the substrate at which the impurity was implanted. Default value and unit: 7°.

tilt.stdev

Standard deviation of the tilt angle for plasma implantation. Default value and unit: 0° .

tolerance

Error tolerance for convergence to extract the dual-Pearson implantation moments from data.file. Default value and unit: 0.1%.

ts4.backscattering

Switches the TS4 backscattering model on or off. In this model, the portion of the profile distribution that sticks out of the solid structure is assumed to be lost, resulting in slightly less dose than the nominal dose. Default: false.

vfactor

Scaling factor for the vacancy profile calculation in the plus.one and frenkel.pair models. It is used for the frenkel.pair model in the case of analytic implantation only. Default: 1.

## **Arguments: Deprecated**

conformality

Specifies the constant conformal doping fraction between 0 and 1:

- conformality=0 is standard implantation.
- conformality=1 is fully conformal doping.

igrid.file

Specifies the file name for storing the damage information in the internal grid of Crystal-TRIM. This is not used in Sentaurus MC.

keepdamage.igrid

Keeps the damage information stored at the internal grid between two runs of Crystal-TRIM. This is not used in Sentaurus MC.

## A: Commands

### implant

`mpp`

Switches on or off the multiprocess parallelization (MPP) feature for Monte Carlo implantations. However, if the pdb parameter ParallelJobs is equal to 1, no parallel jobs will be run even if `mpp` is on. Default: true.

`predamage.igrid`

Uses the damage from the internal grid for a Crystal-TRIM run. This is not used in Sentaurus MC.

`save1d`

Specifies that the 1D profiles as calculated by Sentaurus MC implantation will be saved in (x,y) format. These saved files have the particle names as the file name extension. Valid for 1D or quasi-1D structures only.

`save1d.file`

Specifies the file name for the 1D profiles as calculated by Sentaurus MC implantation. These saved files have the particle names as the file name extension. Valid for 1D or quasi-1D structures only.

`save1d.unit`

Specifies the unit of the x-axis for the 1D profiles as calculated by Sentaurus MC implantation. Valid units are A, nm, and  $\mu$ m.

## Description

There are two main branches to this command. The first allows you to specify models and parameters for analytic implantation. It can be performed by specifying `tables` or `species`. The second performs an implantation into the current structure. Either analytic functions or the Monte Carlo method can be used.

## Examples

Change all implantation specifications for the species boron from the default to the Taurus implantation tables and models:

```
implant species= Boron tables= Taurus
```

Change the default implantation table for boron in silicon to `my_table.tab` and the implantation model to `pearson`. In addition, switch off the damage calculation for boron in silicon:

```
implant species= Boron Silicon imp.table= my_table.tab pearson !damage
```

Specify a 100 keV implantation of phosphorus with a dose of  $1\times10^{14}\text{ cm}^{-2}$ . The previously assigned data files and models are used to obtain range statistics:

```
implant Phosphorus dose= 1e14 energy= 100
```

Specify an implantation of arsenic with a dose of  $1\times10^{15}\text{ cm}^{-2}$  and energy of 60 keV. Use Sentaurus MC simulation. Point-defect profiles will be calculated from the damage profile:

```
implant Arsenic dose= 1e15 energy= 60 sentaurus.mc defect.model= frenkel.pair
```

## See Also

[Chapter 3 on page 53](#)

## A: Commands

init

---

## init

Sets up the mesh and background doping levels.

### Syntax

```
init
  [Adaptive]
  [concentration=<n>] [<m-3>|<cm-3>|<um-3>|<nm-3>]
  [DelayFull1D] [done]
  [field=<c>]
  [fields.values= <list>]
  [load.commands] [<material>]
  [miscut.tilt=<n>] [miscut.toward= {<n> <n> <n>}]
  [notch.direction= <list>]
  [pdb] [pdb.only] [resistivity]
  [sat=<c>] [sigmac=<c>]
  [slice.angle=<n>] [<degree>]
  [tdr=<c>] [top]
  [wafer.orient= <list>]
```

### Arguments

#### Adaptive

When loading a TDR file containing geometry but no mesh, a mesh is generated automatically. This argument determines whether adaptive meshing is used. The default is the return value of `pdbGet Grid Adaptive`.

#### concentration

Concentration of the incorporated data field. The only available unit is  $\text{cm}^{-3}$ , but any nodal quantity (with any internal unit) can be initialized with this argument if no unit is specified. Default value and unit:  $0.0 \text{ cm}^{-3}$ .

#### DelayFull1D

By default, Sentaurus Process generates a minimum-dimensional structure, which will be extruded to higher dimensions when Sentaurus Process encounters a *mask*. To generate a full-dimensional structure, use `!DelayFull1D`.

#### done

Returns 1 if the initialization is performed; otherwise, returns 0.

#### field

Name of the data field to be initialized everywhere in the structure.

fields.values

Specifies a list of parameters where the parameter name is the name of the field to be introduced in the bulk regions of the new structure, and the value is the initial value, for example, `fields.values= {Boron=1e18}`. A list of fields of any name can be initialized with this argument and, for solution variables or stress components, units are accepted.

To initialize mole fractions in alloy materials, you can either use `xMoleFraction` or `yMoleFraction` or both directly, or use the `MoleFractionFields` command (see [MoleFractionFields on page 1089](#)).

load.commands

Loads the commands in the TDR format file. Default: true.

<material>

Specifies a material for doping. It must be used with the `field` argument.

miscut.tilt

Specifies the magnitude of the wafer miscut, that is, the angle between the actual wafer normal and the direction as specified by `wafer.orient`. This argument is used in both analytic and Monte Carlo implantations. Default value and unit: 0° (no wafer miscut).

miscut.toward

Specifies the orientation of the wafer miscut as a list of three Miller indices. That is, the wafer normal moves away from `wafer.orient` by a `miscut.tilt` angle and moves *towards* the `miscut.toward` direction. The actual wafer normal is between the `wafer.orient` and `miscut.toward` directions. This argument is used in both analytic and Monte Carlo implantations. The default value of `miscut.toward` is the same direction as `notch.direction= {1 1 0}`.

notch.direction

**NOTE** This was originally the `flat.orient` argument.

Specifies a direction from the wafer center to the notch using a list of three Miller indices, or specifies an orientation that is normal to the wafer flat (imagine that a wafer flat is a plane parallel to `wafer.orient`). Default: `{1 1 0}`.

pdb

Loads pdb parameters along with geometry and data in the TDR file. Default: true.

## A: Commands

init

`pdb.only`

Loads only pdb parameters without geometry and data in the TDR file. Default: false.

`resistivity`

Sets the value of the field by requesting a resistivity. This argument only works for fields that have the resistivity pdb parameters set (which, by default, are only As, B, P, Sb, and In in silicon).

`sat`

Specifies to read the structure file in the Sentaurus Structure Editor format.

`sigmac`

Specifies to read the structure file in Sigma-C 3D format.

`slice.angle`

Angle of the simulation domain with respect to the wafer coordinate system. Default value and unit:  $-90^\circ$ .

The `slice.angle` can be specified using a `CutLine2D` command:

```
init slice.angle= [CutLine2D 1.65 0.15 1.95 0.6]
```

`tdr`

Specifies the TDR format file to read.

In general, a TDR file can contain a variety of information depending on which tool was used to generate the file. By default, Sentaurus Process writes files with sufficient information to restart a simulation. This includes current parameter settings, stored commands (such as polygon, mask, contact), bulk mesh and data, and, in three dimensions, a boundary (see [Saving a Structure for Restarting Simulations on page 45](#)). If such a file is specified, all this data is read and used to restart the simulation. It is also possible to read TDR files that include only bulk mesh and data, or only a boundary. If only a boundary is available, Sentaurus Process creates a mesh using current refinement criteria. Finally, a TDR file can contain information for restarting a Sentaurus Process KMC simulation. TDR files containing more information can be created by using the `kmc extract tdrAdd` command and the `kmc extract tdrWrite` command (see [kmc on page 1037](#)). However, TDR files generated by Sentaurus Device do not contain information to restart a simulation and may not be read correctly.

For information about the TDR format, refer to the *Sentaurus™ Data Explorer User Guide*.

top

Specifies that the gas is found at the smallest x-value (at the top of the structure). If !top is specified, the gas is added at the highest x-value (at the bottom). Default: true.

wafer.orient

Wafer orientation specified as three Miller indices. Default: wafer.orient= {0 0 1}.

## Description

Sets up the mesh from either a rectangular specification or a file. The command also allows initialization of the background doping concentration and type.

## Examples

Read in a structure previously saved using struct tdr=temp, which produces the file tmp\_fps.tdr:

```
init tdr= temp
```

Create a structure with the current mesh parameters and a uniform boron doping of  $1\times10^{15}$ :

```
init field= Boron concentration= 1e15
```

Initialize a structure and set the Germanium and Silicon fields so that the mole fraction is 0.2, that is, Si<sub>0.8</sub>Ge<sub>0.2</sub>:

```
init fields.values= [MoleFractionFields SiliconGermanium 0.2]
```

Initialize a structure with a (110) wafer and an 8° miscut *towards* the <1̄10> direction:

```
init wafer.orient= {1 1 0} notch.direction= {1 -1 0} miscut.tilt= 8 \
miscut.toward= {1 -1 0}
```

## See Also

[CutLine2D on page 924](#)

[line on page 1053](#)

[MoleFractionFields on page 1089](#)

[region on page 1161](#)

[struct on page 1217](#)

## A: Commands

insert

---

# insert

Inserts segments into 1D structures, polygons into 2D structures, and polyhedra into 3D structures.

## Syntax

```
insert
  polygon=<c> | polyhedron=<c> | segments= {<n1> <n2> ...}
  [Adaptive]
  [fields.values= <list>]
  [new.material=<c>] [new.region=<c>]
  [repair]
  [replace.materials= {<mat1> ... <matn>}]
  [replace.regions= {<reg1> ... <regn>}]
```

## Arguments

Adaptive

If specified, Adaptive switches on adaptive meshing if remeshing. Parameters for adaptive meshing are described in [Adaptive Mesh Refinement on page 729](#). The default is the return value of `pdbGet Grid Adaptive`.

fields.values

Specifies a list of parameters where the parameter name is the name of the field to be introduced in the inserted geometry and the value is the initial value, for example, `fields.values= {Boron=1e18}`. A list of fields of any name can be initialized with this argument and, for solution variables or stress components, units are accepted.

new.material

Sets the material for the inserted segment, polyhedron, or polygon. This argument is mandatory for all but TDR polyhedra or polygons.

new.region

Sets the name of the inserted region. It works with one segment, polygon, or polyhedron only, that is, it does not work if the segment, polygon, or polyhedron contains more than one region.

**NOTE** This argument is not allowed for TDR polyhedra.

`polygon`

Specifies the polygon to insert. Only polygons created with the `xy` argument of the `polygon` command are allowed. The `polygon` argument fails if the simulation is three dimensional, or if it is one dimensional and cannot be extruded to two dimensions because there are no `y`-lines available.

`polyhedron`

Specifies the polyhedron to insert. It needs a 3D simulation or a simulation that can be extruded to three dimensions.

`repair`

If specified, this option enables an algorithm that tries to repair sharp features or geometric artifacts produced by polyhedron insertion. Repair operations can be disabled either globally by setting `mgoals !repair.3d` or locally for each `insert` command by specifying `!repair`. Default: true.

`replace.materials`

Specifies a list that indicates the materials to be replaced by the polyhedron. In addition to explicit materials, the argument `bulk.materials` is allowed. If `bulk.materials` is used, it means that all materials in the structure, except gas, will be replaced.

`replace.regions`

Specifies a list of regions to be replaced by the polyhedron.

`segments`

Segments are defined as a list of an even number of coordinates (in  $\mu\text{m}$ ). If more than two coordinates are specified, unique region names are generated for each segment or region.

## Description

Segments are defined using the `segments` argument, but polygons and polyhedra must be defined using the `polygon` and `polyhedron` commands, respectively. You must specified one of the `segments`, `polyhedron`, or `polygon` arguments.

When specified, `replace.materials` and `replace.regions` provide a list of materials and regions to be replaced. If neither is specified, all materials will be replaced. If both are specified, the union of them will be replaced. The `new.material` argument changes the polyhedron material temporarily.

The `insert` command can be used to perform polyhedron or polygon etching and deposition as well as the more general polyhedron or polygon insert functionality. Polyhedron or polygon etching is performed by specifying `new.material=gas` or by creating a gas polyhedron. You

## A: Commands

### insert

also can do the same in one dimension with `segments`, but this is the same as `CMP` or `fill`. Polyhedron or polygon deposition is performed by specifying `replace.materials=gas` as well as having one or more bulk materials in the polyhedron or polygon, or defining them temporarily with `new.material`.

The `insert` command operates only in the 3D MGOALS mode for polyhedra. If the SDE mode is switched on, calling this command will set `sde off`.

**NOTE** It is recommended that no faces of the polyhedron overlap material interfaces or the outermost simulation boundary. This may cause failures due to round-off errors or may create poor mesh elements such as slivers.

### Examples

Etch the structure using a polyhedron called `prism`:

```
insert polyhedron= prism new.material= Gas
```

Replace all materials in the structure with a polyhedron called `smallCube`, and fill the polyhedron with oxide:

```
insert polyhedron= smallCube new.material= Oxide
```

Replace the nitride, and only the nitride, in the simulation with oxide inside the polyhedron called `smallCube`:

```
insert polyhedron= smallCube replace.materials= {Nitride} new.material= Oxide
```

Replace all materials in the structure with a polygon called `Channel1`, and fill the polygon with material `Silicon2`, and the region is named `ChannelRegion`. This polygon can be inserted without merging with neighboring silicon regions:

```
mater add name= Silicon2 new.like= Silicon alt.matername= Silicon
```

```
insert polygon= Channel new.material= Silicon2 new.region= ChannelRegion
```

### See Also

[Inserting Polyhedra on page 826](#)

[polygon on page 1124](#)

[polyhedron on page 1128](#)

---

# integrate

Returns the volume integration of the named quantity.

## Syntax

```
integrate
  [absolute] [average] [element] [interfaces]
  [<material>]
  [max= {<n> <n> <n>}]
  [min= {<n> <n> <n>}]
  [mode= mesh | boundary | jagged]
  [name=<c>] [region=<c>]
  [skipgas] [syntax.check.value=<c>]
```

## Arguments

absolute

Specifies that integration is performed with the absolute values of the named quantity.

average

Specifies that the average value of the named quantity is computed and added to the returned Tcl list.

element

Specifies that integration is performed elementwise. In this case, it is expected that the quantity specified by name is an elemental quantity.

interfaces

Specifies that integration is performed on interface meshes.

<material>

Used to limit integration to regions of the specified material. See [Specifying Materials on page 18](#).

max

List of numbers defining the x-, y-, and z-coordinates of the lower-right front corner of the cutting box. For 1D, 2D, and 3D structures, a list of one, two, or three numbers is required, respectively. The possible maximum number is used for missing numbers.

## A: Commands

integrate

min

List of numbers defining the x-, y-, and z-coordinates of the upper-left back corner of the cutting box. For 1D, 2D, and 3D structures, a list of one, two, or three numbers is required, respectively. The possible minimum number is used for missing numbers.

mode

Specifies the integration mode within a given box:

- The mesh mode (default) uses a mesh-cutting algorithm.
- The boundary mode for three dimensions cuts the boundary to a cuboid and remeshes the cuboid using the given mesh refinements. The boundary mode is for 3D simulations only.
- The jagged mode includes all nodes contained entirely within the given box for integration.

name

Quantity to be integrated. Default: Z\_Plot\_Var.

region

Limits integration to only the region specified.

skipgas

Specifies that integration is omitted on invisible meshes.

syntax.check.value

Sets a value to be returned only during syntax-checking mode. Sometimes, the value returned by a command can cause a false syntax-check error because the value returned by the command would not be the value during the normal run mode. Setting this value avoids such problems.

## Description

This command integrates the field specified with the name argument (by default, the last unnamed select command field) over the entire structure or within a given box specified by min and max. If material is specified, the integration is limited to regions of the given material. If a region is specified, the integration is limited to only the named region.

The command by default expects the quantity to be nodal and the integration is performed nodewise, but if element is given, an elemental quantity is expected and the integration proceeds elementwise.

A Tcl list is returned where the first value is the integrated value.

The second value is the volume of the computed regions:

- In  $\text{<value\_unit>}^*\text{cm}$  for one dimension
- In  $\text{<value\_unit>}^*\text{cm}^2$  for two dimensions
- In  $\text{<value\_unit>}^*\text{cm}^3$  for three dimensions

where  $\text{<value\_unit>}$  is the unit of the named quantity.

The third value is the dose (the integrated value divided by the simulated area in  $\text{cm}^{-2}$  in all dimensions). The fourth and fifth values are the minimum and maximum of the named quantity, respectively. If average is specified, the averaged result for the named quantity is appended to the returned Tcl list.

## Examples

Return the integral boron in all silicon regions in the structure, the volume of all silicon regions, and the combined boron dose in all silicon regions:

```
integrate silicon name= Boron
```

Return the integrated pressure elementwise in the entire structure (excluding gas) and the volume of the structure (excluding gas):

```
select z= "1.0/3*(StressEL_xx+StressEL_yy+StressEL_zz)"  
integrate element
```

Return a list of integral, volume, dose, minimum, maximum, and average values of boron within the box defined by the upper-left corner (0.0, 0.0) and the lower-right corner (10.0, 0.2):

```
integrate name= Boron average min= {0. 0.} max= {10. 0.2}
```

Return the integrated term BActive, the volume, and the combined dose in all silicon regions in the structure. The term BActive is first converted to a temporary data field before integration:

```
select z= BActive  
integrate silicon
```

Return a list of integral, volume, dose, minimum, and maximum of boron within the cuboid defined by the upper-left back corner (0.0, 0.0, 0.0) and the lower-right front corner (0.4, 0.4, 0.4):

```
integrate name= Boron mode= jagged min= {0. 0. 0.} max= {0.4 0.4 0.4}
```

## interface

Returns the location or the value of the selected data field at a material interface.

### Syntax

```
interface
  [All] [data] [<material>] [name=<c>]
  [p1= {<n> <n> <n>} p2= {<n> <n> <n>}] 
  [precision=<n>]
  [region=<c>]
  [side=<c>]
  [syntax.check.value=<c>]
  [thickness]
  [x=<n>] [<m>|<cm>|<um>|<nm>]
  [y=<n>] [<m>|<cm>|<um>|<nm>]
  [z=<n>] [<m>|<cm>|<um>|<nm>]
```

### Arguments

All

If specified, all interface locations are returned. Otherwise, only the first value is returned.

data

If specified, the value of the selected data field at the interface is returned.

<material>

Usually works with an interface description and returns the location or value of the selected quantity at the interface. See [Specifying Materials on page 18](#). When the thickness option is specified, a material name can be used.

**NOTE** If the thickness option is not specified *and* an interface is not specified, an error occurs. If the specified interface does not exist in the current structure, an error is reported.

name

Name of the data field to be returned when data is specified. Default: Z\_Plot\_Var.

p1, p2

Specify the two endpoints of a cutline. Both p1 and p2 must be specified together as a list of numeric values. Only the first <dim> numbers from each list is read, where <dim> is the spatial dimension of the simulation. Specifying the endpoints with p1 and p2 allows for

nonaxis-aligned cuts. Endpoints also can be used to limit axis-aligned cuts instead of cutting through the entire structure.

#### precision

Controls the number of precision digits of floating values (in scientific notation). Default: 6.

#### region

When the `thickness` option is specified, you can specify the name of a region from which to extract its thickness.

#### side

Takes its value from one of the two bulk materials consisting of the interface or the ‘interface’ (literally) itself. If `side` is not specified, the ‘interface’ itself is assumed. If `side` is specified as one of the bulk materials, the value of the selected data field for the bulk material is returned. This argument is effective only if `data` is specified.

#### syntax.check.value

Sets a value to be returned only during syntax-checking mode. Sometimes, the value returned by a command can cause a false syntax-check error because the value returned by the command would not be the value during the normal run mode. Setting this value avoids such problems.

#### thickness

Specify this option to extract the thickness of a region. The thickness of the first region along the cutline will be returned. The unit of the returned thickness is micrometer. When you specify this option, you can specify a material or region, but not an interface. If a material is specified, the thickness of the first material region will be returned. If a region is specified, the thickness of the region will be returned.

#### x, y, z

Provide the description of a line to look for the interface. These arguments are unnecessary in 1D simulations. In 2D simulations, one of `x` and `y` must be specified. In 3D simulations, two of these must be specified. Default value and unit: 0.0  $\mu\text{m}$ .

## Description

This command returns the position of an interface or returns the value of the selected data field if `data` is specified. Therefore, the command can be used to prepare plots of material thickness, silicon consumption, or material growth. It also is used to provide an argument to the `interpolate` command, which returns a list if there is more than one interface. The list-processing commands of Tcl, particularly `lindex`, are very helpful.

## A: Commands

### interface

#### Examples

Return the silicon–oxide interface at a lateral position of 1.0  $\mu\text{m}$ :

```
interface y= 1.0 silicon /oxide
```

Return the top position of the oxide:

```
interface oxide /gas
```

Return any oxide–nitride interfaces between (1.0, 1.0) and (1.1, 1.1). This specification is valid for one or two dimensions, but not three dimensions. In one dimension, it returns the interfaces between 1.0 and 1.1:

```
interface p1= {1.0 1.0} p2= {1.1 1.1} Nitride /Oxide
```

#### See Also

[interpolate on page 1033](#)

[plot.xy on page 1118](#)

[point.xy on page 1122](#)

---

## interpolate

Returns the requested position or value at a specified location.

### Syntax

```
interpolate
<material> [name=<c>]
[syntax.check.value=<c>]
[value=<n>]
[x=<n>] [<m>|<cm>|<um>|<nmm>]
[y=<n>] [<m>|<cm>|<um>|<nmm>]
[z=<n>] [<m>|<cm>|<um>|<nmm>]
```

### Arguments

<material>

Limits the search to a single material. See [Specifying Materials on page 18](#).

name

Name of a data field. This allows printing without using the `select` or `tclsel` commands. Default: `Z_Plot_Var`.

syntax.check.value

Sets a value to be returned only during syntax-checking mode. Sometimes, the value returned by a command can cause a false syntax-check error because the value returned by the command would not be the value during the normal run mode. Setting this value avoids such problems.

value, x, y, z

The combination of these arguments determines how the command operates:

- In 1D simulations, you must supply either `x` or `value`. If `x` is supplied, Sentaurus Process returns the value at `x`. If `value` is supplied, Sentaurus Process returns the locations at which the selected profile crosses `value`.
- In 2D simulations, two of the four arguments must be given (not `z`).
- In 3D simulations, three of the four arguments must be given.

For example, in two dimensions, if `x` and `value` are given, the locations along `x` where `value` is crossed are returned. If `x` and `y` are given, the value at the location (`x,y`) is returned. The default unit of `x`, `y`, and `z` is  $\mu\text{m}$ .

## A: Commands

interpolate

### Description

This powerful command analyzes simulation results. It returns the interpolated value of one coordinate given the other two coordinates in three dimensions defined by x- and y-variables, and the data field. It also works for 1D simulations by returning values as a function of one coordinate.

This command returns a Tcl list of values if more than one is found. For example, there may be several junctions found along a given line. All of these are returned and can be processed by standard Tcl list operations. In most cases, this command returns a single value. The returned value is in internal units. Internal units are CGS; for example, the unit for stress is  $\text{dyn}/\text{cm}^2$ .

In addition, this command can return the data value at a specified position in the structure or return the position at which a specified data value occurs.

### Examples

Return the value of the data field at the position ( $1.0 \mu\text{m}$ ,  $1.0 \mu\text{m}$ ) in the oxide:

```
interpolate oxide x= 1.0 y= 1.0
```

Return a list of zero crossings in silicon of the data field along the vertical line  $y = 0.0 \mu\text{m}$ :

```
interpolate y= 0.0 silicon value= 0.0
```

Return a list of zero crossings in silicon along a horizontal line at a depth of  $2.0 \mu\text{m}$ :

```
interpolate silicon x= 2.0 value= 0.0
```

Return the value of the data field at  $1.0 \mu\text{m}$ :

```
interpolate x= 1.0 silicon
```

Return the yy component of the element stress field at  $1.0 \mu\text{m}$ :

```
interpolate x= 1.0 oxide name= StressEL_yy
```

Return a list of zero crossings in silicon material:

```
interpolate silicon value= 0.0
```

### See Also

[interface on page 1030](#)  
[plot.xy on page 1118](#)  
[point.xy on page 1122](#)

---

## KG2E

Computes Young's modulus from the bulk modulus and the shear modulus.

### Syntax

KG2E <n> <n>

### Arguments

<n>

The first value is the bulk modulus.

The second value is the shear modulus.

### Description

The same units are assumed for all moduli.

### Examples

Compute Young's modulus from the bulk modulus 1.2272e12 dyn/cm<sup>2</sup> and the shear modulus 6.328e11 dyn/cm<sup>2</sup>:

KG2E 1.2272e12 6.328e11

**A: Commands**KG2nu

---

## KG2nu

Computes the Poisson ratio from the bulk modulus and the shear modulus.

### Syntax

```
KG2nu <n> <n>
```

### Arguments

<n>

The first value is the bulk modulus.

The second value is the shear modulus.

### Description

The same units are assumed for all moduli.

### Examples

Compute the Poisson ratio from the bulk modulus 1.2272e12 dyn/cm<sup>2</sup> and the shear modulus 6.328e11 dyn/cm<sup>2</sup>:

```
KG2nu 1.2272e12 6.328e11
```

---

## kmc

Specifies options for the atomistic kinetic Monte Carlo (KMC) mode.

### Syntax

```

kmc
  add |
  add queue name=<c> [amorphous | crystalline] [clustertype name=<c>]
    [coordx=<n>] [<m>|<cm>|<um>|<nm>]
    [coordy=<n>] [<m>|<cm>|<um>|<nm>]
    [coordz=<n>] [<m>|<cm>|<um>|<nm>] |
  deatomize name=<c> [active] [<material>] |
  defects.read=<c> |
  defects.write=<c> [defectname=<c>] [materialname=<c>] |
  defecttypes [<material>] |
  (extract
    acinterface
      [coordx=<n>] [<m>|<cm>|<um>|<nm>]
      [coordy=<n>] [<m>|<cm>|<um>|<nm>]
      [coordz=<n>] [<m>|<cm>|<um>|<nm>] |
    defects
      [name=<c>] ([acinterface] [detailed])
      [countdefects] [countparticles]
      [defectname=<c>] [materialname=<c>] |
    dose [countdefects] [defectname=<c>] [materialname=<c>] [name=<c>] |
    histogram name=<c> [materialname=<c>] [meansize [minsize=<n>]] |
    materials
      [coordx=<n>] [<m>|<cm>|<um>|<nm>]
      [coordy=<n>] [<m>|<cm>|<um>|<nm>]
      [coordz=<n>] [<m>|<cm>|<um>|<nm>] [detailed] |
    profile
      name=<c>
      [coordx=<n>] [<m>|<cm>|<um>|<nm>]
      [coordy=<n>] [<m>|<cm>|<um>|<nm>]
      [coordz=<n>] [<m>|<cm>|<um>|<nm>]
      [defectname=<c>] [materialname=<c>] [timeaveraged] |
    supersaturation [name=<c>] |
    tdrAdd [concentrations] ([defects] | [visual= <list>]) [histogram]
      [list= <list>] [Stress] |
    tdrClear |
    tdrWrite [filename=<c>]) |
  materialtypes | off | particletypes | PDEupdated | present [name=<c>] |
  remesh | report

```

## A: Commands

kmc

### Arguments

acinterface

The kmc extract acinterface command returns the 1D coordinates of the amorphous–crystalline transitions present in the simulation. If the simulation has  $N$  dimension, it needs  $N - 1$  cutlines, specified by coordx, coordy, or coordz.

The kmc extract defects acinterface command returns the atomistic position of lattice atoms in the amorphous–crystalline interface, when using the LKMC recrystallization mode.

active

Used by kmc deatomize to deatomize only the active part of a dopant.

add

Instructs Sentaurus Process KMC to add a new defect into the simulation cell. The defect to be included must be first sent to the queue using kmc add queue. Here, the defect is specified with name, and the coordinates with coordx, coordy, and coordz. When all defects are in the queue, the command kmc add, without any arguments, passes the defects from the queue to Sentaurus Process KMC, erasing the queue.

amorphous, crystalline

When added to kmc add, amorphous creates the defect and changes the material to amorphous.

When used with kmc add, crystalline creates the defect in a crystalline phase of the material, locally recrystallizing the area where the defect will be added when necessary.

clustertype

Defines the type of defect specified in name. For example, kmc add queue clustertype name=I56 returns if this cluster is considered an amorphous pocket (AP), a {311}, or a loop.

concentrations

Instructs Sentaurus Process KMC to generate concentration information to be included in the TDR file. It is used with kmc extract tdrAdd.

coordx, coordy, coordz

Specify the x-, y-, and z-coordinates needed for the kmc add queue command. They also are used to specify the cutlines in the kmc extract profile and kmc extract materials commands. Default unit:  $\mu\text{m}$ .

**countdefects**

Used with kmc extract defects to instruct Sentaurus Process KMC to count the number of defects instead of listing the particles in the defects.

Used with kmc extract dose to compute the dose of defects, not particles. For example, the dose of loops is different from the dose of particles in loops.

**countparticles**

Used with kmc extract defects to instruct Sentaurus Process KMC to count and return the number of particles, instead of listing them.

**deatomize**

Instructs Sentaurus Process KMC to build a new data field and fill it with the concentrations taken from the KMC simulation. name is the field to create. For deatomize, the argument name also can be XTotal or NetActive, where X means any dopant. It accepts the active argument to account for the active part of the dopant only.

**defectname**

Specifies an optional name of a defect (for example, ThreeOneOne, ImpurityCluster) for:

- kmc defects.write=<c>
- kmc extract defects
- kmc extract dose
- kmc extract profile

This argument is used to further refine name. For example, if name=I, using defectname refines these interstitials to interstitials as point defects, or in impurity clusters, and so on.

**defects**

kmc extract defects returns the defects currently present in the simulation.

kmc extract tdrAdd defects appends to the TDR file an atomistic 3D view of the defects currently contained in the simulation, allowing for visualization, and loading and continuing the simulation.

**defects.read**

Specifies the name of a text file from which to read its defects and to insert them in the current simulation.

## A: Commands

kmc

defects.write

Specifies the name of a text file into which to write all the current defects in the simulation.  
Use defectname and materialname to filter the defects written.

defecttypes

Using kmc defecttypes returns the name of the defects that can be used by defectname.

detailed

Produces different results depending on the context:

- kmc materials detailed returns the current list of materials for each internal KMC element, including the element coordinates.
- kmc extract defects acinterface detailed works as kmc extract defects acinterface, but returns all the lattice atoms in the LKMC model, and not solely those belonging to the amorphous–crystalline interface.

dose

Using kmc extract dose returns doses (concentration in  $\text{cm}^{-2}$ ). The argument countdefects returns the dose of defects, instead of the dose of particles (which is the default). The defects and particles included in this dose are refined with name and defectname.

extract

kmc extract retrieves information about the current status of the KMC simulation. This information is mainly concentrations, histograms, the atomistic positions of defects, and the types of defect. kmc extract also controls the information written to the TDR file.

It is mandatory to use another argument with kmc extract:

- acinterface returns the 1D coordinates of the amorphous–crystalline transitions present in the simulation.
- defects returns the current list of particles in the simulation.
- dose computes and returns the dose of given particles or defects or both.
- histogram retrieves the number of defects depending on their size.
- materials retrieves the materials currently in the simulation.
- profile returns the concentration of particles, defects, electrons, and holes in the simulation or any cutline of the simulation.

- `supersaturation` returns the concentration relative to equilibrium for interstitials and vacancies.
- `tdrAdd`, `tdrClear`, and `tdrWrite` control the information to be written to the TDR file.

`filename`

Specifies the name of the TDR file to be written by `kmc extract tdrWrite`.

`histogram`

`kmc extract histogram` returns the number of defects for each defect size. The argument `name` determines the returned histogram. If `name` is `XI` or `XV` (`X` being a dopant or impurity), it returns the histogram of impurity clusters for that dopant with `Is` or `Vs`. If the name is `I` or `V`, it produces the histogram of `I` or `V` extended defects. Finally, if `name=IV`, it returns the AP histograms.

If `meansize` is included, the returned value is not a list of defects and sizes, but the average size for these defects. The minimum size for computing this average is zero by default, but it can be changed using `minsize`.

`kmc extract tdrAdd histogram` includes histogram information in the TDR file.

`list`

Adds a list of fields to be included in the TDR file. This argument is used in `kmc extract tdrAdd`. Any specific defect name is allowed, and generic defect names (as obtained by `kmc defecttypes`) also are allowed. For example, `I8` adds this cluster to the TDR file, but `AmorphousPockets` adds any AP existing in the simulation.

`<material>`

Specifies the material name for `kmc deatomize` or `kmc defecttypes`. See [Specifying Materials on page 18](#).

`materialname`

Restricts the output to the material specified. `materialname` adds a condition to the output of `kmc extract defects`, `profile`, `dose`, and `histogram`.

`materials`

`kmc extract materials` returns a list of materials currently present in the simulation.

`kmc extract materials detailed` returns the coordinates and the materials of the KMC elements.

## A: Commands

kmc

materialtypes

Returns the subset of materials allowed in the Sentaurus Process KMC simulation. Any material not listed here is assigned as ‘unknown’.

meansize

Used only with kmc extract histogram. It instructs Sentaurus Process KMC to compute the average size for the specified defect type. The minimum size needed to take the defect into account is 0, unless minsiz e is specified.

minsize

Used only with kmc extract histogram meansize. It instructs Sentaurus Process KMC to use the specified value as the minimum size to take any cluster into consideration when computing the average cluster size.

name

Specifies the name of the field, particle, or defect for the following arguments. In the following, *X* is the name of a valid dopant (such as B or As). *Any defect* means very detailed defects such as  $B_2I_3$ ,  $I_8$ ,  $I_4V_5$ , and  $AsV_4$ . *Any particle* means point defects, dopants, impurities, or impurity- and dopant-paired point defects in any charge state, that is, any name obtained with kmc partictypes (for example, I, VMM, BiP, or F):

- add is the name of the defect or particle to be added. XAmorphous and XIInterface also are acceptable.
- clustertype is any defect.
- deatomize is any defect or any particle. XAmorphous, XIInterface, XTotal, NetActive, pNetActive, nNetActive, and tNetActive also are valid.
- defects is any defect or any particle.
- dose is any defect or any particle.
- histogram: XI, XV, I, V, and IV are the only valid names.
- present is any defect or any particle. XAmorphous, XIInterface, and XTotal also are valid.
- profile is any defect or any particle. Holes, electrons, XAmorphous, and XIInterface also are valid.
- supersaturation allows only I or V.

off

Use kmc off to delete the Sentaurus Process KMC information and to remove the current KMC object from memory.

**NOTE** Use with caution.

particletypes

Returns a list of valid particle names. This list may change between simulations, depending on the dopants specified in the parameter database.

PDEupdated

Returns true if the state of Sentaurus Process KMC did not change since the last time the PDEs were synchronized (by using KMC2PDE).

present

Returns true when the species specified in name is in the KMC simulation.

profile

Using kmc extract profile returns concentrations. These concentrations contain 1D, 2D, or 3D information depending on the simulation dimension. Cutlines can be specified with coordx, coordy, and coordz. Each of these arguments reduces the dimensions of the output by 1. The concentrations in 1D simulations can be directly compared with SIMS profiles.

The argument name specifies the particle or defect from which the concentration is obtained. If name is a valid particle name (see particletypes), defectname can be used with a valid defect name (see defecttypes) to further refine name. When a particle is specified using name, profile returns the concentration of particles; otherwise, it returns the concentration of defects.

Some particular names that can be used are:

- electrons, holes, Bandgap (or gap), GapNarrowing, Fermi\_level, and ni for electronic concentrations.
- stressXX, stressXY, stressZZ, strainXX, strainYY, strainZZ, strainXY, strainXZ, and strainYZ for mechanical properties.
- dopants for the net active concentration.
- Ge for the germanium concentration.

## A: Commands

kmc

queue

Adds the new defect, specified by name, into the simulation at the coordinates coordx, coordy, and coordz. Adding defects to the queue will not put them in the KMC simulation. To transfer the defects from the queue to the simulation, use kmc add without any other arguments.

remesh

Instructs Sentaurus Process KMC to remesh the structure. This remesh is especially helpful in the hybrid mode, where the Sentaurus Process KMC structure is not updated automatically during certain process steps, such as etch and strip. Therefore, defect or particle information from any region that has been removed during the step is not updated until this command is called. You should call the kmc remesh command immediately after such a process step.

report

Instructs Sentaurus Process KMC to generate a list of defects created during the simulation. This list includes the first and last time the defect was seen and the temperature. If the defect is still in the simulation, the report also gives the number of defects. In addition, a report is printed automatically at the end of the diffuse and implant commands.

Stress

Using kmc extract tdrAdd Stress adds the stress and strain distribution as imported by Sentaurus Process KMC.

supersaturation

Using kmc extract supersaturation returns the value of the global supersaturation (concentration over equilibrium concentration). The argument name must be specified; it can only be *I* or *V*.

tdrAdd

Using kmc extract tdrAdd instructs Sentaurus Process KMC to add a new *snapshot* of information ready to be written into a TDR file. This information is stored in memory and is written using kmc extract tdrWrite. In addition, kmc extract tdrAdd without arguments adds an empty snapshot. The tdrAdd options are:

- concentrations computes and adds 1D, 2D, or 3D concentrations for each particle and defect.
- defects adds atomistic 3D information. It allows you to see the shape and position of the defect, and to load and continue the simulation.
- histogram adds histograms for extended defects and impurity clusters.

- `list` adds user-specified defects. For example, `concentrations` only adds ‘I in ThreeOneOne’, but `list` can be used to add `I45`, `I65`, and so on. Specifying the name of a defect (as obtained in `kmc defecttypes`) adds all the clusters in this particular defect for each existing size in the simulation.
- `stress` includes stress fields in the file.
- `visual` includes atomistic information for visualization purposes in the file.

#### `tdrClear`

`kmc extract tdrClear` removes all snapshots previously added using `kmc extract tdrAdd` from memory.

#### `tdrWrite`

`kmc extract tdrWrite` instructs Sentaurus Process KMC to write all snapshots (previously added using `tdrAdd`) to a file. The name of the file is specified using `filename`.

#### `timeaveraged`

Must be used with `kmc extract profile`. It generates time-averaged concentrations of particles, instead of instantaneous ones. The averaging is performed between two snapshots. Since `timeaveraged` only makes sense for mobile particles, the argument `name` must be a valid particle *not* a defect.

#### `visual`

When added to `kmc extract tdrAdd`, it includes atomistic information that can be used for visualization purposes only, and not for restarting (in contrast with `kmc extract defects`).

`visual` attempts to produce a file as small as possible without losing atomistic information. You must specify a list of the type of defects to be saved. Generic defects (such as `ThreeOneOne`, `Void`), specific ones (such as `B2I3`), or materials (`Silicon`) specified act as filters for the defects to be saved.

To save all of them, use `visual=all`.

### Description

This command sends direct instructions to Sentaurus Process Kinetic Monte Carlo (Sentaurus Process KMC), which is used for diffusion. The main options are:

- `add` creates defects in the simulation.
- `deatomize` creates fields according to the atomistic concentrations.

## A: Commands

kmc

- `extract` returns physical information (mainly concentrations) about the simulation. It has different arguments including `defects`, `dose`, `histogram`, `profile`, `tdrAdd`, `tdrClear`, and `tdrWrite`.

## Examples

Create an  $I_8$  cluster, a mobile  $B$  in interstitial position, and the BIC  $B_2I_2$  in the queue, and add the queue to the KMC simulation:

```
kmc add queue coordx= 10<nm> coordy= 15<nm> coordz= 6<nm> name= I8  
kmc add queue coordx= 3<nm> coordy= 8<nm> coordz= 7<nm> name= B2I2  
kmc add queue coordx= 5<nm> coordy= 5<nm> coordz= 5<nm> name= Bi  
kmc add
```

Return whether an  $I_{543}$  is a ThreeOneOne or a loop in this simulation:

```
kmc clustertype name= I543
```

Create a `BTotAl` data field, which will be computed by Sentaurus Process KMC including all the boron in any defect in the simulation:

```
kmc deatomize name= BTotAl
```

Create an  $As_4V$  data field, filled with the  $As_4V$  information taken from the KMC simulation:

```
kmc deatomize name= As4V
```

Return a list of the different defect types modeled by Sentaurus Process KMC:

```
kmc defecttypes
```

Return a list containing the particles currently in the KMC simulation, including its defect type, defect number, and coordinates. Particles with the same defect number belong to the same defect:

```
kmc extract defects
```

Return a list of each  $I$  particle currently in the KMC simulation:

```
kmc extract defects name= I
```

Return the  $B$  particles in impurity clusters currently in the simulation:

```
kmc extract defects name= B defectname= ImpurityCluster
```

Return the number of particles in  $B_2I_3$  defects:

```
kmc extract defects name= B2I3 countparticles
```

Return the number of  $B_2I_3$  defects in the simulation:

```
kmc extract defects name= B2I3 countdefects
```

Return a list of particles currently in the KMC simulation. It also returns the ‘hidden’ particles, which are regenerated by Sentaurus Process KMC using internal information (see [Damage Accumulation Model: Amorphous Pockets on page 428](#)):

```
kmc extract defects detailed
```

Return the  $As_4V$  defects present in the simulation:

```
kmc extract defects name= As4V
```

Return the electron concentration computed by Sentaurus Process KMC:

```
kmc extract profile name= electrons
```

Return the BIC histograms:

```
kmc extract histogram name= BI
```

Return the average size of I in extended defects. The minimum size to be included in this average is set to 40:

```
kmc extract histogram name= I minsizes= 40
```

Return the concentration of  $I_2V_3$  defects:

```
kmc extract profile name= I2V3
```

Return the concentration of holes in the KMC simulation:

```
kmc extract profile name= holes
```

Return the concentration of boron in any defect:

```
kmc extract profile name= B
```

Return the concentration of substitutional boron:

```
kmc extract profile name= B defectname= PointDefect
```

Return the dose (concentration in  $cm^{-2}$ ) of interstitials in {311}s:

```
kmc extract dose name= I defectname= ThreeOneOne
```

Return the list of materials currently present in the simulation:

```
kmc extract materials
```

## A: Commands

kmc

Return the coordinates of each KMC element and its material:

```
kmc extract materials detailed
```

Return the concentration of mobile interstitials in the simulation:

```
kmc extract profile timeaveraged name= I
```

Return the interstitial supersaturation:

```
kmc extract supersaturation name= I
```

Clear all the previous stored information, add a new snapshot with the concentration of particles and the atomistic information for any defect, and write the information in a TDR file called example.tdr. Since defects is included, this file also can be used to load and continue the simulation:

```
kmc extract tdrClear  
kmc extract tdrAdd concentrations defects  
kmc extract tdrWrite filename= example.tdr
```

Return the list of materials supported by Sentaurus Process KMC:

```
kmc materialtypes
```

Return the list of particles supported by Sentaurus Process KMC. This list can be changed using pdb commands:

```
kmc particletypes
```

Return true (1) or false (0) depending on the presence of BI<sub>2</sub> in the simulation:

```
kmc present name= BI2
```

Exit Sentaurus Process KMC and remove all its associated information from memory:

```
kmc off
```

Print a list of the simulated defects with the first and last time they were seen and the temperature in the simulation:

```
kmc report
```

In one dimension, return the concentration of B<sub>2</sub>I<sub>2</sub> at x = 10 nm. In two dimensions, return the concentration of B<sub>2</sub>I<sub>2</sub> in the line x = 10 nm. In three dimensions, return the concentration of B<sub>2</sub>I<sub>2</sub> in the plane x = 10 nm:

```
kmc extract profile name= B2I2 coordx= 10<nm>
```

Return the concentration in the line y with x = 10 nm and z = 15 nm:

```
kmc extract profile name= B2I2 coordx= 10<nm> coordz= 15<nm>
```

Create a TDR snapshot with any {311} defect and the BI<sub>2</sub> and B<sub>2</sub>I<sub>2</sub> defects:

```
kmc extract tdrAdd list= {ThreeOneOne BI2 B2I2}
```

## See Also

[Chapter 5 on page 373](#)  
[deposit on page 928](#)  
[diffuse on page 935](#)  
[etch on page 952](#)  
[implant on page 1001](#)  
[integrate on page 1027](#)  
[line on page 1053](#)  
[photo on page 1109](#)  
[profile on page 1137](#)  
[region on page 1161](#)  
[select on page 1168](#)  
[stressdata on page 1209](#)  
[struct on page 1217](#)

---

## KMC2PDE

Translates atomistic KMC information to Sentaurus Process.

### Syntax

KMC2PDE

### Description

This command translates the atomistic information stored in the KMC diffusion into continuum five-stream quantities and transfers it into the standard Sentaurus Process mesh. Consequently, there are two transformation involved here:

- Deatomization of particles into concentrations
- Translation of Sentaurus Process KMC field names into Sentaurus Process field names

The deatomization is performed in a standard way by calling `kmc deatomize` for each existing Sentaurus Process KMC field. If the Sentaurus Process mesh is too coarse, the continuum fields will look smooth, but some information may be lost. On the other hand, if the Sentaurus Process mesh is too fine, isolated islands of concentration may form following its corresponding atomistic concentrations.

The translation is made as accurately as possible by mapping as many KMC species into similar five-stream fields. When this one-to-one mapping is not possible or not unique, acceptable approximations can be taken. For example, `Bi` will be translated into `BoronInt`, but `B2I2`, `BI2`, and so on will be translated into only `BCluster`. A complete list of these translations is available in the file `KMC.tcl`.

### See Also

[UnsetAtomistic on page 1252](#)

---

# layers

Prints material interfaces and integrated data field values.

## Syntax

```
layers
  [<material>] [merge] [name]
  [precision=<n>] [print.logfile]
  [region.names] [syntax.check.value=<c>]
  [x=<n>] [<m>|<cm>|<um>|<nm>]
  [y=<n>] [<m>|<cm>|<um>|<nm>]
  [z=<n>] [<m>|<cm>|<um>|<nm>]
```

## Arguments

<material>

Used to limit the reporting of layers to regions of the specified material. See [Specifying Materials on page 18](#).

merge

Specifies that the adjacent regions with the same material should be merged. Default: false.

name

Name of a data field. This allows printing without using the select or tclsel commands. Default: Z\_Plot\_Var.

precision

Controls the number of precision digits of floating values (in scientific notation). Default: 12.

print.logfile

Allows output to be written to the log file.

region.names

Specifies that region names must be printed in addition to the material names for each region in the structure.

## A: Commands

layers

syntax.check.value

Sets a value to be returned only during syntax-checking mode. Sometimes, the value returned by a command can cause a false syntax-check error because the value returned by the command would not be the value during the normal run mode. Setting this value avoids such problems.

x, y, z

Specify the constant values of a line along which sectioning will be performed. In one dimension, these arguments are not necessary. In two dimensions, only one of x or y can be specified for a given device. Specifying x produces a horizontal slice through the device, and y specifies a vertical slice. An easy way to remember this is that the cross section is taken at the constant value specified. For a 3D simulation, two of these three arguments must be specified. Default unit:  $\mu\text{m}$ .

### Description

This command prints the material interfaces and integrates the selected data field in each region. It is most useful for examining doping because it gives the integrated doping in each layer. This command can be simulated with the `integrate` and `interface` commands, and it returns a Tcl list of each material.

### Examples

In a 1D simulation, list all material interfaces:

layers

In a 2D simulation, list all material interfaces at a lateral position of 0.0  $\mu\text{m}$  and integrate the data field named Boron:

layers y= 0.0 name= Boron

### See Also

[integrate on page 1027](#)

[interface on page 1030](#)

[select on page 1168](#)

[tclsel on page 1222](#)

---

## line

Specifies the position and spacing of mesh lines.

### Syntax

```
line
  location=<n> [<m> | <cm> | <um> | <nm>] (x | y | z)
  [clear] [kmc] [mgoals]
  [spacing=<n>] [<m> | <cm> | <um> | <nm>]
  [spacing.method= even | regular | smooth]
  [tag=<c>] [virtual.spacing]
```

### Arguments

clear

Clears lines in preparation for a new structure definition, or removes all ticks stored for the UseLines method (see [UseLines: Keeping User-Defined Mesh Lines on page 756](#)).

kmc, mgoals

Lines for KMC and Sentaurus Mesh (continuum) meshes are stored separately. By default, line commands are applied to both KMC and continuum meshes. Use negative values for these arguments to *not* apply mesh lines to one or the other. For example, for a line command to apply only to a continuum mesh, use !kmc.

location

Location along the chosen axis. Default unit:  $\mu\text{m}$ .

spacing

Local grid spacing. Each mesh line has a characteristic required spacing. Lines are graded from one spacing to the next over the interval. The default is a spacing equal to the largest interval between the neighboring lines. Default unit:  $\mu\text{m}$ .

spacing.method

Specifies the method to use when distributing the ticks created by the spacing argument:

- even: Distributes the ticks evenly, trying to approximate the spacing specified at the beginning of the interval.
- regular: Distributes the ticks evenly using the exact spacing specified at the beginning of the interval, and leaving the last interval with an approximate size if there is no more room to accommodate the requested size.

## A: Commands

### line

- **smooth:** Distributes the ticks to have a smooth grading of spacing between lines.

Default: `smooth`.

#### tag

Lines can be labeled for later reference by `region` commands. The label can be any word.

#### virtual.spacing

If specified, this option enables the creation of virtual ticks between lines. The mesh refinement will snap to these virtual ticks whenever possible. When Sentaurus Mesh attempts to produce a refinement that is finer than the spacing provided by the virtual ticks, it will proceed to split the spacing in half using the default bisection algorithm.

#### x, y, z

Orientation of the mesh line. Specifying `x` places a mesh line at a constant `x`-value. A series of `line x` commands would specify the horizontal grid locations during the simulation.

## Description

The `line` command is used with the `init` and `region` commands to create the initial mesh. Only rectilinear structures can be specified with the `line` and `region` commands, that is, rectangular regions in two dimensions and cuboid-shaped regions in three dimensions.

Sentaurus Process uses the unified coordinate system (UCS):

- `x` is the direction normal to the wafer with positive-`x` oriented into the bulk of wafer.
- `y` is perpendicular to the `x`-direction and lies along the wafer surface; `y` is in the lateral direction.
- The `z`-direction is used for three dimensions, and the direction is given by  $X \times Y$ .

By default, Sentaurus Process delays promoting a structure until it is necessary (by use of a higher dimensional mask). The lines specifying the higher dimensions are stored until they are needed. During the `init` command, the `line` and `spacing` information is expanded into mesh ‘ticks’ that are stored in the PDB. These ticks are used every time a mesh is created if `UseLines` is switched on (see [UseLines: Keeping User-Defined Mesh Lines on page 756](#)).

When you specify the `spacing` argument, the `line` command generates a series of lines or ticks that is incorporated into the mesh refinement as lines that completely cut through the device. This is useful to generate the spacing for the initial structures generated by the `init` and the `region` commands. After the `init` command, however, if new lines are specified and `UseLines` is switched on, the `spacing` argument is ignored, and only one tick or mesh line can be added at a time.

However, if the `virtual.spacing` option is specified, the `spacing` argument will be used to build a series of *soft* lines or ticks. All user-defined refinement coordinates will snap to those lines, thereby creating a more predictable spacing pattern compared to the one generated by the default bisection algorithm.

To create an entirely new structure, the command `line clear` must first be issued to remove old lines and mesh ticks before issuing new `line`, `region`, and `init` commands.

## Examples

There are three user-specified y-lines and two user-specified x-lines. Taking the y-lines as an example, there is a finer spacing in the center than at the edges. After processing, Sentaurus Process produces a mesh with x-lines at 0.0, 0.42, 0.69, 0.88, 1.0, 1.12, 1.31, 1.58, and 2.0. Around the center, the spacing is 0.12, approximately what will be requested. At the edge, the spacing is 0.42 because that is as coarse as it could become without having an interval ratio greater than 1.5 (a fixed quantity). If the interval ratio was allowed to be 9, for example, there would be one interval of 0.9 and one interval of 0.1 on each side. In this example, specifying a spacing of 1 at the edges is redundant because that is what the spacing of the user-specified lines was already:

```
line x location= 0 spacing= 0.02 tag= surf
line x location= 3 spacing= 0.5 tag= back
line y location= 0 spacing= 1 tag= left
line y location= 1 spacing= 0.1
line y location= 2 spacing= 1 tag= right
```

In the following example, a structure with two bricks is created using the `line` and `region` commands. After the structure is created, a set of virtual lines is enabled to guide the refinement. If the `virtual.spacing` option is not used, the default bisection algorithm would place the refinement at powers of 2 between the given line locations:

```
mgoals accuracy=0.002

line x loc=0.0 spacing=0.1 tag=top
line x loc=0.2 spacing=0.1 tag=siflat
line x loc=1.0 spacing=0.1 tag=bottom
line y loc=0.0 spacing=0.1 tag=left
line y loc=0.1 spacing=0.1 tag=mid
line y loc=0.2 spacing=0.1 tag=right

region Silicon xlo=siflat xhi=bottom
region Silicon xlo=top xhi=siflat ylo=left yhi=mid

init !DelayFullD

line clear
line virtual.spacing
line x loc=0.0 spacing=0.01
line x loc=0.2 spacing=0.01
```

## A: Commands

line

```
line x loc=1.0 spacing=0.01
line y loc=0.0 spacing=0.01
line y loc=0.1 spacing=0.01
line y loc=0.2 spacing=0.01

refinebox clear
refinebox xrefine = 0.1 yrefine = 0.1
refinebox interface.materials = Silicon min.normal.size = 0.0075 \
    normal.growth.ratio = 1.5

deposit oxide iso thickness =0.1
struct tdr=virtualspacing
```

### See Also

[init on page 1020](#)  
[region on page 1161](#)

---

## line\_edge\_roughness

Adds line edge roughness (LER) to named masks.

### Syntax

```
line_edge_roughness
    correlation.length=<n> [<m> | <cm> | <um> | <nm>]
    masks= <list>
    max.segment.length=<n> [<m> | <cm> | <um> | <nm>]
    normal= "Y" | "Z"
    standard.deviation=<n> [<m> | <cm> | <um> | <nm>]
    [max.tries=<n>] [min.radius=<n>]
    [random.reseed] [random.seed=<n>] [smooth.points=<n>]
```

### Arguments

correlation.length

Specifies the correlation length of the randomized LER. Corresponds approximately to the concept of *wavelength*. Default value and unit: 20  $\mu\text{m}$ .

masks

Specifies as a list the names of masks to receive LER defined by the other arguments in the line\_edge\_roughness command.

max.segment.length

Specifies the maximum segment length. Mask edges are subdivided into segments that are approximately this size or smaller before LER deviation is added to each. Default value and unit: 1  $\mu\text{m}$ .

max.tries

Specifies the maximum number of LER mask generation attempts. For nonzero values, detection of nearly collinear points is performed after LER generation, and the LER process is restarted if decimation occurs based on the `mgoals` accuracy value. The default value is 0, meaning that the LER mask is accepted as it is, with no decimation detection.

min.radius

When `normal` is not specified, where two mask edges receiving LER meet, the corner is first rounded before LER is applied. This allows a well-defined application of LER and avoids discontinuous jumps in the resulting mask shape. The rounding radius is the greater of `min.radius` and twice the `correlation.length`. Default unit:  $\mu\text{m}$ .

## A: Commands

line\_edge\_roughness

normal

Defines the normal axis. Only mask segments normal to this axis receive LER. This axis is also the reference axis along which the LER deviation is added to the given mask segment. The default is to add LER to all edges of the mask.

random.reseed

Before the calculation of LER, the random number generator is reseeded to ensure each call of line\_edge\_roughness results in randomized noise that is uncorrelated with other calls of line\_edge\_roughness.

To switch off random reseeding, use !random.reseed to reproduce the same LER from call to call. Default: true.

random.seed

Used to reproduce specific LER calculations from one run to the next by setting the same random seed in both runs. Ignored when !random.reseed is used.

smooth.points

Alters the LER function at the structure boundaries, allowing for better mirror boundary conditions when uniting symmetry-reduced structure parts at those boundaries. Defines the number of segments in the discrete LER function, counting from the boundary edge of the mask, which must be adjusted or smoothed. Default: 0 (implying no smoothing).

standard.deviation

Specifies the standard deviation of the randomized LER. Corresponds approximately to the concept of added noise *amplitude*. Default value and unit: 2  $\mu\text{m}$ .

## Description

This command adds LER to the named masks, along the mask edges normal to the given normal axis ("Y" or "Z"). LER can be added to a mask only once. See [Boolean Masks on page 806](#).

## Examples

Add LER to the mask named mask1 along mask segments normal to the z-axis. These segments are subdivided into smaller segments of length smaller than or equal to 5 nm. LER is characterized by a correlation.length of 25 nm and standard.deviation of 5 nm. The random number generator is reseeded automatically before LER is calculated:

```
line_edge_roughness normal= "Z" masks= {mask1} \
    correlation.length= 25.00<nm> standard.deviation= 5.00<nm> \
    max.segment.length= 5.00<nm>
```

## See Also

[Line Edge Roughness Effect on page 807](#)

---

# load

Interpolates data from a TDR file onto the current mesh.

## Syntax

```
load
  tdr=<c> (merge | rename | replace | sum)
  [fast.tdr.ave= <list>]
  [flip (left | right | front | back | up | down)]
  [keep.outside] [material.specific] [offset= {<n> <n>}]
  [save.transform=<c>]
  [shift=<n>]
  [species= <list> actions= <list>]
  [transform= {<n> <n> <n> <n> <n> <n>}]
```

## Arguments

`fast.tdr.ave`

Averages the data from a list of TDR files (all with identical meshes to the current mesh) and replaces the current data with the averaged data from the files.

**NOTE** Do not use `fast.tdr.ave` with any other argument. To use it, specify a list of files, for example:

```
fast.tdr.ave= {mydata1.tdr mydata2.tdr mydata3.tdr}
```

`flip (left | right | front | back | up | down)`

Performs a flip of the data in the indicated direction about the outer boundary before interpolation. This argument must be used with a direction, for example, `flip front`.

`keep.outside`

Specifies that the fields outside the bounding box of the loaded TDR file will remain unchanged. If this option is switched off (false) and the `replace` option is specified, the fields outside the TDR bounding box will be deleted (assuming the TDR bounding box is smaller than the current device bounding box). Default: false.

## A: Commands

load

material.specific

By default, interpolation is material specific, so that data is interpolated from the file if the material in the existing structure matches. Use !material.specific to allow interpolation regardless of material.

merge

Adds only new datasets that do not currently exist in the structure.

offset

For 2D structures only. Offsets the data by a vector before loading it.

rename

Adds new datasets and renames them by adding the suffix \_\_load.

replace

Adds new datasets and replaces existing datasets with new datasets of the same name.

save.transform

Saves a TDR file for the transformed structure. You can examine the saved TDR file to ensure the loaded structure is in the required location.

shift

Shifts the data laterally before loading it.

species, actions

These lists specify field-by-field actions. The field name must be one of those in the loaded TDR file. The actions in the actions list can be merge, rename, replace, and sum.

sum

Adds new datasets and sums matching datasets.

tdr

Specifies the name of the command file in the TDR format. Sentaurus Process checks for standard file names with the .tdr extension. For 2D structures, a 3D TDR command file is also allowed. The data on the 2D overlap cross-section between the 3D structure and the 2D structure will be interpolated to the current 2D mesh. When calculating the intersection, the 2D structure is assumed to be located at z=0.

**transform**

Provides a general interface for translating or rotating the structure to be loaded before interpolation. When loading 3D results to a 2D structure, since the 2D structure is assumed to be located at z=0, to obtain 3D data other than on the cross section at z=0 of the 3D structure, this argument can be used to transform the 3D structure to a required location.

In one dimension, one value must be specified: the shift in the x-coordinate.

In two dimensions, six values must be specified: rxx, ryx, rxy, ryy, offsetx, offsety.

In three dimensions, 12 values must be specified: rxx, ryx, rzx, rxy, ryy, rzy, rxz, ryz, rzz, offsetx, offsety, and offsetz. First, the offset is applied, and then the rotation matrix is applied. Sentaurus Process uses a right-hand coordinate system, so the rotation must follow the right-hand rule and the rotation matrix should be specified correctly. For example, in three dimensions, for a 90° rotation about the x-axis, the rotation matrix should have rxx=1, rzy=-1, ryz=1, and the remaining values should be zero.

**Description**

This command interpolates data from TDR files onto the current mesh. There are several options for handling the new and old datasets. First, the actions can be applied individually to selected datasets using `species` and `actions`. If the `species` list appears, the `actions` list must be specified and must have the same number of members as the `species` list. If this is the case, only the `species` in the `species` list are taken from the external datasets. If the `species` list does not appear, one of the global actions is used. The default behavior is a global sum where new datasets are added and, if there is an existing dataset with the same name, the external data is added (summed) with the existing dataset.

The other actions that can be performed are:

- `merge` takes only the new datasets that do not currently exist in the structure.
- `rename` renames new datasets by appending `_load` to the name, which can be manipulated with the `select` command as required.
- `replace` replaces current datasets with new datasets of the same name.
- In atomistic mode, only `tdr` and `replace` can be used to replace the current simulation contents with the particles stored in a TDR file.

**Examples**

Replace all existing datasets with those in the file `in_fps.tdr`:

```
load tdr= in replace
```

**A: Commands**

load

Load the TDR file `in_fps.tdr`, sum `Arsenic_Implant` and the existing `Arsenic_Implant` (if available), and replace the existing `Damage_Implant` data field by the one in the `in_fps.tdr` file:

```
load tdr= in species= {Arsenic_Implant Damage_Implant} actions= {sum replace}
```

**See Also**

[select on page 1168](#)

---

## LogFile

Prints a message to the screen and to the log file.

### Syntax

```
LogFile
<C>
[IL0 | IL1 | IL2 | IL3] [PrintCommands]
```

### Arguments

<C>

Specifies the message to be printed to the screen and to the log file.

IL0, IL1, IL2, IL3

Specifies the information level.

PrintCommands

Specifies whether commands are printed to both the screen and the log file. To stop the printing of commands, use !PrintCommands. Default: true.

### Description

This command prints messages to the terminal window in which Sentaurus Process is running and to the log file. If IL0, IL1, IL2, or IL3 is given and this command is called from within a Sentaurus Process command, the message is printed only if the information level is equal to or greater than the one specified.

### Examples

Print the string "Step 25" to the screen and the log file:

```
LogFile "Step 25"
```

Print the contents of the Tcl variable DebugInfo only if info=1 or higher has been specified in the calling command:

```
LogFile IL1 "$DebugInfo"
```

## A: Commands

### LogFile

Do not print the `sel z=1e10 name=Test` command and subsequent commands to the screen and the log file:

```
LogFile !PrintCommands  
sel z=1e10 name=Test
```

---

## mask

Creates a mask for subsequent use in `etch`, `deposit`, or `photo` commands.

### Syntax

```
mask
  [bbox] [bool=<c>] [clear] [covered.status]
  [cut.x=<n> (materials= <list> | regions= <list>)]
  [get.segments] [get.segments.z]
  [list] [name=<c>] [negative]
  (
    [polygons= <list>] [segments= <list>] |
    [left=<n>] [<m>|<cm>|<um>|<nm>]
    [right=<n>] [<m>|<cm>|<um>|<nm>]
    [front=<n>] [<m>|<cm>|<um>|<nm>]
    [back=<n>] [<m>|<cm>|<um>|<nm>]
  )
)
```

### Arguments

`bbox`

Returns the mask bounding box. The command returns a list of lists where the values are in centimeters: {`ymin zmin`} {`ymax zmax`}.

`bool`

Performs Boolean operations between masks. It cannot be used with `polygons` and `negative`. See [Boolean Masks on page 806](#).

`clear`

Clears the list of all masks. If `name` is specified, it clears only that mask.

`covered.status`

Used to obtain information about the coverage of the simulation domain. The following strings may be returned:

- `covered`: The mask completely covers the simulation domain.
- `uncovered`: The mask does not cover the simulation domain at all.

## A: Commands

### mask

- `partial.2d`: The mask partially covers the domain, but in a way that the mask does not promote the simulation dimension (that is, the mask does not vary in the z-direction over the simulation domain).
- `partial`: The mask partially covers the simulation domain, and its use in etching or deposition forces the simulation to three dimensions.

### `cut.x, materials, regions`

The `cut.x` argument is only available in two dimensions. It must be used with either `regions` or `materials` to create a mask. The mask is created by taking a cut through the set of regions created by a union of regions listed in `regions` and regions of one of the materials listed in `materials`. The cut is taken at the x-coordinate specified by `cut.x`, and the resulting outline is used to create the mask. Default unit of `cut.x`:  $\mu\text{m}$ .

### `get.segments, get.segments.z`

Retrieves segments that result from cutting the mask at  $z=\text{get.segments.z}$ . The default value of `get.segments.z` is the midpoint of the simulation domain in the z-direction.

### `left, right, front, back`

Specify the corners of one rectangle. The rectangle is added to the current list for the mask. If several rectangles must be specified for a mask, several `mask` commands must be used with the same name. Default unit:  $\mu\text{m}$ .

### `list`

Prints a list of all currently defined masks. If `name` is specified, it prints information for that mask only.

### `name`

Name of a mask. If used with `clear` or `list`, only the specified mask will be reported or removed. If defining a new mask, `name` must be specified.

### `negative`

Inverts the type of mask. By default, points inside the mask are considered masked. For example, the command `mask name=xyz negative` inverts an existing mask `xyz`.

For an empty negative mask, all points are considered masked, and the simulation domain is fully covered by the mask.

### `polygons`

Specifies a mask as a list of named polygons. The named polygons must have been defined using `polygon` commands.

segments

Specifies a list of coordinates of mask segments. Several mask segments can be specified at the same time. The first coordinate defines the beginning of a segment, the second coordinate defines the end of the segment, the third defines the beginning of the second segment, and so on. In 3D simulations, mask segments are extended across the entire structure in the z-direction. Default unit:  $\mu\text{m}$ .

## Description

This command manages and creates masks for use with subsequent `etch`, `deposit`, or `photo` commands. Mask definitions are stored in TDR files and re-stored when loading a TDR file in the `init` command. Masks can be defined by rectangles, polygons, and segments, or they can be read using the IC WorkBench Edit/View Plus–TCAD Sentaurus interface (see [Chapter 13 on page 835](#)).

Masks are created additively. If more than one `mask` command is issued with the same name, the union of the specified masks is assumed. To change a mask, first clear it and then assign a new specification (in two separate calls to the `mask` command).

## Examples

Define a mask named `field`:

```
mask name= field left= 0.0 right= 10.0
```

The position of this mask is the same as in the previous example:

```
mask name= mgoals segments= {0.0 10.0}
```

Return information about all masks in array format:

```
mask list
```

Return a list of mask names:

```
array set maskinfo [mask list]
LogFile "Mask names: [array names maskInfo]"
```

Print all information about the mask named `PolygonMask`:

```
array set polyInfo $maskInfo(PolygonMask)
LogFile "Contents of PolygonMask: [array names polyInfo]"
```

Print the number of polygons in the mask named `PolygonMask`:

```
LogFile "Number of polygons in PolygonMask: [llength $polyInfo(polygons)]"
```

## A: Commands

### mask

Print the first polygon in the mask named PolygonMask:

```
LogFile "polygon 0 in PolygonMask: [lindex $polyInfo(polygons) 0]"
```

### See Also

[deposit on page 928](#)  
[etch on page 952](#)  
[photo on page 1109](#)  
[point on page 1120](#)  
[polygon on page 1124](#)

## mater

Returns a list of all materials in the current structure, and adds new materials to a global list.

### Syntax

```
mater
  [add]  [alt.matername=<c>]
  [bbox | bbox.cm | bbox.um]  [cropped.bbox]
  [cubic | hexagonal | orthorhombic]
  [horizontal.orient= {<n> <n> <n>}]
  [Interface]  [kmc.shortname=<c>]
  [lattice.const=<n>]  [lattice.const.b=<n>]  [lattice.const.c=<n>]
  [like.interpolate]  [list.all]
  [max= {<n> <n> <n>}]  [min= {<n> <n> <n>}]
  [name=<c>]  [new.like=<c>]
  [polytype=<c>]
  [syntax.check.value=<c>]
  [vertical.orient= {<n> <n> <n>}]
```

### Arguments

#### add

Adds a new material specified by name to the global material list.

#### alt.matername

Specifies the name of the material that should be written in the TDR file for regions of the newly defined material.

For example, when writing the TDR file, if the newly defined material is called MySilicon and alt.matername=Silicon, Sentaurus Process uses Silicon for those regions of MySilicon.

This is useful when transferring the structure to device simulation.

#### bbox, bbox.cm, bbox.um

If specified, the mater command returns the maximum extents of the material in two points in centimeter or micrometer.

#### cropped.bbox

Returns the cropped bounding box of a material within a user-defined bounding box.

## A: Commands

mater

cubic, hexagonal, orthorhombic

Specifies the lattice system as either cubic, hexagonal, or orthorhombic for a crystalline material as specified by name.

horizontal.orient

Specifies the flat orientation for crystalline material as three Miller indices. The default value of horizontal.orient depends on the wafer orientation:

- If vertical.orient= {0 0 1}, horizontal.orient= {1 1 0}.
- If vertical.orient= {1 1 0} or {1 1 1}, horizontal.orient= {1 -1 0}.

For all other nonstandard wafer orientations, a flat orientation that is orthogonal to the wafer orientation must be specified.

**NOTE** The arguments horizontal.orient and vertical.orient supersede notch.direction and wafer.orient specified in the init command for this particular material (as specified by name).

Interface

Returns a list of interface materials in the current structure.

kmc.shortname

Specifies a short name for a parameter for Sentaurus Process KMC.

**NOTE** The kmc.shortname argument must be specified if you intend to change the ShortName parameter for use in Sentaurus Process KMC. This enables setting up the interface parameters with the user-specified ShortName.

lattice.const

Specifies the lattice constant for the crystalline material. Default value and unit:  $5.431 \times 10^{-4}$   $\mu\text{m}$ .

lattice.const.b

Specifies the lattice constant  $b$  for the crystalline material. If lattice.const.b is not specified, it is assumed to be the same as lattice.const. Default unit:  $\mu\text{m}$ .

lattice.const.c

Specifies the lattice constant  $c$  for the crystalline material. If lattice.const.c is not specified, it is assumed to be the same as lattice.const. Default unit:  $\mu\text{m}$ .

like.interpolate

Usually, the interpolation code interpolates data from and to materials that are *like* each other. Use !like.interpolate to prevent such interpolation. See [Like Materials: Material Parameter Inheritance on page 24](#).

list.all

Lists all the materials defined.

max, min

Specify the bounding box of a material. These arguments compute the cropped bounding box of a material.

name

Name of the material.

new.like

Name of the existing material from which all default values are inherited. For newly created materials, pdb parameters for this material are checked first and, if not found, the ‘Like’ material parameters are used (see [Like Materials: Material Parameter Inheritance on page 24](#)).

polytype

Specifies the polytype for the crystalline material as specified by name. For cubic or orthorhombic lattice systems, the valid polytypes are Sc, Bcc, Fcc, and Zincblende. For a hexagonal lattice system, the valid polytypes are 2H, 3C, 4H, and 6H.

syntax.check.value

Sets a value to be returned only during syntax-checking mode. Sometimes, the value returned by a command can cause a false syntax-check error because the value returned by the command would not be the value during the normal run mode. Setting this value avoids such problems.

vertical.orient

Specifies the wafer orientation for crystalline material as three Miller indices. Default value: vertical.orient= {0 0 1}.

**NOTE** The arguments vertical.orient and horizontal.orient supersede wafer.orient and notch.direction specified in the init command for this particular material (as specified by name).

## A: Commands

mater

### Description

This command returns a list of all materials in the current structure. The format of the list is compatible with the material specification for the program. Bulk material names are returned if no arguments are given. Interface materials can be obtained by using `Interface`.

This command also computes the cropped bounding box of a material that lies within a user-specified bounding box defined by `max` and `min`. The `name` argument is given as input.

### Examples

Add germanium material to the global material list and make it inherit the default values from silicon material:

```
mater add name= Germanium new.like= Silicon
```

Specify the crystal properties for hexagonal GaN:

```
mater name= GaN hexagonal polytype= 2H \
lattice.const= 3.189e-4 lattice.const.c= 5.185e-4 \
vertical.orient= {0 0 1} horizontal.orient= {1 1 0}
```

---

## math

Sets the numeric and matrix parameters. Parameters set with the `math` command are stored in TDR files by default.

### Syntax

```
math
[AMS.NegErrCntrl] [FTS.NegErrCntrl] [LocTrnErrCntrl] [NegErrCntrl]
[auto | compatible]
[diffuse | Flow]
[dimension= 1 | 2 | 3]
[extrapolate]
[pardiso | ils] [scale]

[fullNewton | modNewton]
[newtonDeriv] [newtonRate1=<n>] [newtonRate2=<n>]
[newtonStats=<i>] [newtonSteps1=<i>] [newtonTries1=<i>]

[coord.dfise]
[coord.transform coord.translate (coord.read | coord.write)]
[coord.ucs] [coord.xyz] [coord.yxz] [coord.-zyx]

[maxNumberOfDomains=<i>]
[NumberOfElementsPerDomain=<i>]
[numThreads=<i>]
[numThreadsAssembly=<i>]
[numThreadsBoxMethod=<i>]
[numThreadsDeatomize=<i>]
[numThreadsILS=<i>]
[numThreadsImp3d=<i>]
[numThreadsInterp=<i>]
[numThreadsKMC=<i>]
[numThreadsMC=<i>]
[numThreadsMGoals=<i>]
[numThreadsPardiso=<i>]
[numThreadsSano=<i>]
[numThreadsSnMesh=<i>]
[numThreadsTopo=<i>]
[parallel.license= go.serial | go.abort | go.keep | go.recheck | go.wait]
[threadStackSize=<i>]

[milne | difference] [tr_bdf | euler]
[use.interpolated.geom.coeff] [voronoitriangle]
```

## A: Commands

math

### Arguments: Solver Selection

AMS .NegErrCntrl

Allows stricter error control for each solve time step after an adaptive meshing step by calculating the error from negative updates instead of damped results.

auto, compatible

These options modify the conditional numerical reproducibility (CNR) for Intel CPUs. Floating-point computations on an Intel processor might not give bit-for-bit identical results for equivalent computations, even though the same hardware and binary are used. The fused multiply-add (FMA) instruction is a common source of differences. A small difference can be amplified in applications where the boundary moves (for example, oxidation). Therefore, differences can be minimized by specifying the compatible option. Default: compatible.

**NOTE** The CNR value can be set only at the beginning of the simulation before any arithmetic operation is performed. The compatible mode can significantly degrade the performance of the simulation if the PARDISO solver is used.

diffuse, Flow

Specifies the type of equation to which the command specification applies. If omitted, it applies to all equation types.

dimension

Specifies the dimensionality to which the command specification applies. If omitted, it applies to all dimensions.

extrapolate

If this option is specified, extrapolated solutions can be used as the initial guess for the backward differentiation formula (BDF) step. Extrapolated solutions are calculated using solutions at the previous time step and at the first trapezoidal rule (TR1) step.

FTS .NegErrCntrl

Allows stricter error control for the first solve time step by calculating the error from negative updates instead of damped results.

### LocTrnErrCntrl

Allows stricter error control for each solve time step by modifying the handling of negative updates:

- 1 (|upd|/org\*lte+abs)
- 0 (|upd|/org+lte\*abs)

LocTrnErrCntrl can be switched on for individual solution variables in specific materials using:

```
pdbSetBoolean <mater> <solution> LocTrnErrCntrl 1
```

### NegErrCntrl

Allows stricter error control at each Newton iteration step by calculating the error from negative updates instead of damped results. NegErrCntrl can be switched on for individual solution variables in specific materials using:

```
pdbSetBoolean <mater> <solution> NegErrCntrl 1
```

### pardiso, ils

Specifies the type of linear solver to apply to the system:

- pardiso selects the parallel direct solver PARDISO, which is based on the LU factorization with pivoting of the matrix. PARDISO decomposes the matrix.
- ils selects the iterative linear solver ILS, including preconditioners, iterative methods, scaling, and convergence criteria. (You can change the default settings of ILS parameters by specifying pdbSet Math commands.) To set ILS parameters in the parameter database, see [Setting Parameters of the Iterative Solver ILS on page 884](#).

### scale

Applies row/column scaling to the matrix in an attempt to make it better conditioned. This is a recommended argument. No scaling is performed if the modified Newton scheme (modNewton) is used.

## Arguments: Newton Method

### fullNewton, modNewton

Specifies the type of nonlinear equation solver to use:

- fullNewton performs a matrix factorization at each step.
- modNewton tries to reuse one matrix factorization for several solve steps.

## A: Commands

math

The full Newton method may be more robust, but it can use more solution time than the modified Newton method:

- `modNewton` is the default in two dimensions for both PARDISO and ILS.
- `modNewton` is the default for ILS in three dimensions.

`newtonDeriv`

Allows the Jacobian computation to be switched on during the modified Newton step.  
Default: false.

`newtonRate1`

For the modified Newton method, if the solution for any of the Newton steps 1 through `newtonSteps1` is `newtonRate1` or more times better than the previous step, the next step can be a solve-only step. Otherwise, the next step will perform a matrix factorization.  
Default: 4.0.

`newtonRate2`

For the modified Newton method, if the solution for any of the Newton steps `newtonSteps1+1` onwards is `newtonRate2` or more times better than the previous step, the next step can be a solve-only step. Otherwise, the next step will perform a matrix factorization. Default: 32.0.

`newtonStats`

Prints information on Newton iterations.

`newtonSteps1`

For the modified Newton method, any of the Newton steps 1 through `newtonSteps1` must improve the solution by the factor `newtonRate1` over the previous step. Otherwise, the next step will be a full Newton step. For Newton steps `newtonSteps1+1` onwards, the solution at each step must improve by the factor `newtonRate2`. Otherwise, the next step will be a full Newton step. Default: 12.

`newtonTries1`

Number of first modified Newton step breakdowns allowed before switching to the full Newton method. Default: 2.

## Arguments: Time Discretization

`milne`, `difference`

Controls whether the next time step is estimated using the Milne's device or the divided difference method. Default: `milne`.

tr\_bdf, euler

Specifies the type of time discretization scheme to use. The options are TR-BDF(2) or the backward Euler method. Default: tr\_bdf.

## Arguments: Parallel Processing

Sentaurus Process provides parallel processing for Monte Carlo implantation, interpolation, 3D analytic implantation, the KMC charge model, the matrix assembly, the box method, and the linear solvers by generating multiple threads to accelerate simulations on multicore shared-memory computers. By default, only one processor (thread) is used.

**NOTE** The number of threads must not exceed the number of actual CPUs (cores) of the computer.

**NOTE** Observe the following general recommendations to obtain the best results from a parallel run: Speedup is only obtained for sufficiently large problems. In general, the mesh should have at least 10000 nodes. Three-dimensional problems are good candidates for parallelization.

**NOTE** You must run a parallel job on an unloaded computer. As soon as multiple jobs compete for processors, performance decreases significantly (a parallel job could run even longer than a serial one).

**NOTE** The parallel execution of the matrix assembly on the solvers PARDISO and ILS produces different rounding errors. Therefore, the number of Newton iterations in particular may change.

**NOTE** Parallel performance scalability of the different modules (such as assembly and linear solver) can vary dramatically.

**NOTE** You do not need to set the OpenMP environment variable OMP\_NUM\_THREADS. You need only specify the number of threads required in the math command.

To use more than one thread, specify the following arguments of the math command in the command file:

maxNumberOfDomains

Modifies the maximum number of domains each level of partition can have (see [Partitioning and Parallel Matrix Assembly on page 887](#)).

## A: Commands

math

NumberOfElementsPerDomain

Modifies the number of elements that must go to each domain (see [Partitioning and Parallel Matrix Assembly on page 887](#)).

numThreads

Specifies the number of parallel threads for Sentaurus Process. Applies to Sentaurus MC implantation, interpolation, 3D analytic implantation, Sentaurus Process KMC, matrix assembly, the box method, and the solvers PARDISO and ILS.

To run MGOALS, Sentaurus Process KMC, matrix assembly, the box method, or the solvers with a different number of threads, specify the following arguments:

- numThreadsAssembly
- numThreadsBoxMethod
- numThreadsDeatomize
- numThreadsILS
- numThreadsImp3d
- numThreadsInterp
- numThreadsKMC
- numThreadsMC
- numThreadsMGoals
- numThreadsPardiso
- numThreadsSano
- numThreadsSnMesh
- numThreadsTopo

Separately, these arguments have priority over numThreads.

numThreadsAssembly

Number of threads used for matrix assembly. Parallel assembly of the matrix applies only to inert anneals.

numThreadsBoxMethod

Number of threads used for the box method.

numThreadsDeatomize

Number of threads used when deatomizing KMC particles into continuum finite-element fields.

numThreadsILS

Number of threads for the ILS solver.

Improved parallel implementations of a default diffusion iterative solver `gmres` can be activated by the command:

```
pdbSet Math diffuse <2D | 3D> ILS.hpc.mode <0 | 1 | 2 | 3 | 4>
```

For the high-performance computing mode, the options are 4 (default), and the algorithmic parallel enhancements are activated by:

- 1 for Version E-2010.12
- 2 for Versions F-2011.09 and G-2012.06
- 3 for Versions H-2013.03 and I-2013.12
- 4 for Versions J-2014.09, K-2015.06, L-2016.03, M-2016.12, and N-2017.09

numThreadsImp3d

Number of threads used for 3D analytic implantation.

numThreadsInterp

Number of threads used for interpolation. Because of the memory-intensive nature of interpolation, the performance benefit of multithreading may saturate, but it depends strongly on the simulation. If you observe saturation, reduce the value of this argument.

numThreadsKMC

Number of threads used for Sentaurus Process KMC diffusion.

**NOTE** Parallelism for Sentaurus Process KMC only works for 1D or 2D Sentaurus Process simulations.

numThreadsMC

Number of threads used for Sentaurus MC implantation. This value is overwritten by `numThreadsKMC` if it is specified.

numThreadsMGoals

Number of threads used for MGOALS-related operations.

## A: Commands

math

numThreadsPardiso

Number of threads when running PARDISO.

numThreadsSano

Number of threads used for the Sano method for KMC particle to finite-element field smoothing computation.

numThreadsSnMesh

Number of threads used when running Sentaurus Mesh.

numThreadsTopo

Number of threads used when calling Sentaurus Topography to perform etching and deposition steps.

parallel.license

If you run a simulation in parallel mode but the number of parallel licenses is insufficient, Sentaurus Process proceeds in serial mode (default behavior or if `parallel.license=go.serial` is specified), or waits for parallel licenses (`parallel.license=go.wait`), or aborts (`parallel.license=go.abort`). The option `parallel.license=go.recheck` checks for parallel licenses at each parallel step, regardless of whether or not the licenses were available at the previous step.

If `parallel.license=go.keep`, Sentaurus Process checks out a number of parallel licenses using the current value of `numThreads=<i>` at the next parallel step, but it will not return the parallel licenses to the server until the end of the simulation flow. In other words, the subsequent parallel license check will be disabled, and all modules will use the same number of parallel licenses in the entire run.

**NOTE** When the parallel licenses have been checked out, the new command `math numThreads=<i>` will not change the number of parallel licenses currently in use.

threadStackSize

Stack size for each thread. Default stack size is  $2^{18} = 262144$  bytes (see [Partitioning and Parallel Matrix Assembly on page 887](#)).

## Arguments: Coordinate System Input and Output Selection

coord.dfise

Reads or writes files using the DF-ISE coordinate system. This must be used only to revert coordinate systems. If the dimension of the structure changes, `math coord.dfise` must be recalled.

coord.transform, coord.translate, coord.read, coord.write

Both coord.transform and coord.translate allow a general coordinate transformation through specification of a rotation matrix defined as follows:

coord.transform= {a11 a12 a13 a21 a22 a23 a31 a32 a33}

where  $a_{ij}$  ( $i = \text{row}$ ,  $j = \text{column}$ ) are the members of the rotation matrix, and:

coord.translate= {x y z}

specifies a translation vector.

Both coord.transform and coord.translate must be used with either coord.read or coord.write to indicate the transformation is specifying the transformation for reading or writing, respectively. When specifying coord.write, the inverse of the specified transformation is applied when reading. When coord.read is specified, the inverse transformation is applied when writing.

coord.ucs, coord.xyz

Reads and writes files in the UCS.

coord.yxz

Same as coord.dfise in two dimensions.

coord.-zyx

Same as coord.dfise in three dimensions.

### Arguments: General

use.interpolated.geom.coeff

Switches on the method to be used for interpolating geometric coefficients for TRBDF, which reduces the number of box method calls by one third.

voronoitriangle

Switches on the internal box method calculation.

### Description

This command is used to specify the:

- Different coordinate systems.
- Number of threads and the arguments used for parallel processing on shared-memory computers.
- Default options on the matrix packages to be used for different equations.

## A: Commands

math

- Arguments for the Newton method.
- Different time discretization schemes.

### Examples

Use the ILS solver for mechanics in the 2D case:

```
math flow dim= 2 ils
```

Use the PARDISO solver with two threads for the PDE system in the 2D case and specify nested dissection (ND) ordering for PARDISO:

```
math diffuse dim= 2 pardiso numThreadsPardiso= 2 scale  
pdbSetDouble Pardiso.Ordering 2
```

**NOTE** To run in parallel mode, the solvers PARDISO and ILS must be used with ND ordering for both the 2D and 3D cases. For example, to specify ND ordering, use:

```
pdbSetDouble Pardiso.Ordering 2  
pdbSet Math diffuse 2D ILS.symmOrdering nd
```

Select the solver ILS for all equations in two dimensions. Print Newton statistics at the end of each diffuse command. In the first case, the modified Newton method and the TR-BFDF(2) methods are used. In the second case, the Euler and the full Newton methods are specified:

```
math dimension= 2 ils newtonStats= 1  
math dimension= 2 ils newtonStats= 1 euler fullNewton
```

---

## mgoals

Modifies the default parameters for geometric operations available in the MGOALS module.

### Syntax

```
mgoals
[accuracy=<n>] [<m>|<cm>|<um>|<nm>]
[analytic.thickness=<n>] [<m>|<cm>|<um>|<nm>]
[aniso.etching.fragment.tol=<n>]
[aniso.etching.protect.materials]
[dx=<n> dy=<n> dz=<n>]
[fill.buried] [fill.buried.interface=<material>]
[fill.buried.match.surrounding]
[force.analytic | force.full.levelset | force.full.levelset.depo | 
    force.full.levelset.etch]
[fourier.local.diffusivity]
[full.resolution=<n>]
[keep.closed.voids]
[max.number.levelset.cells=<n>]
[min.gas.thickness=<n>] [<m>|<cm>|<um>|<nm>]
[min.levelset.size=<n>] [<m>|<cm>|<um>|<nm>]
[print.params]
[reinitfrequency=<n>] [reinititerations=<n>]
[remove.floating.regions]
[repair.2d] [repair.2d.deposit] [repair.2d.etch] [repair.2d.photo]
[repair.3d] [repair.3d.deposit] [repair.3d.etch] [repair.3d.photo]
[repair.angle=<n>] [repair.crystal.depo.facets]
[resolution=<n>]
[trapezoidal.algorithm=<n>] [use.brep.2d]
[M-2016.12-SP2 | M-2016.12-SP1 | M-2016.12 | L-2016.03-SP2 | L-2016.03-SP1 |
    L-2016.03 | K-2015.06-SP2 | K-2015.06-SP1 | K-2015.06 | J-2014.09-SP2 |
    J-2014.09-SP1 | J-2014.09 | I-2013.12-SP2 | I-2013.12-SP1 | I-2013.12 |
    H-2013.03-SP2 | H-2013.03-SP1 | H-2013.03 | G-2012.06-SP2 | G-2012.06 |
    F-2011.09-SP1 | F-2011.09 | E-2010.12 | D-2010.03]
```

### Arguments

#### accuracy

Specifies the error that can be tolerated in transferring the new interface definition from the level-set grid to the simulation grid. There is a compromise between smoothness and the number of grid points. Smoother grids need more points on curved regions. Default value and unit:  $1.0 \times 10^{-5} \mu\text{m}$ .

## A: Commands

mgoals

`analytic.thickness`

For etching and deposition steps of layers of thickness of 1 nm or less, an analytic method performs the etching because thin etches using the level-set method can be prohibitively CPU and memory intensive.

For very large or very small structures, a 1-nm cutoff may be inappropriate, so this argument can be used to modify the thickness where the analytic method is used. Default unit:  $\mu\text{m}$ .

`aniso.etching.fragment.tol`

Removes fragments remaining from 3D anisotropic etching. The tolerance measures the ratio of the volume and the surface of a region. Default: 1.0e-6.

`aniso.etching.protect.materials`

When switched on, the 3D anisotropic algorithm attempts to protect areas shadowed by buried materials. Default: false.

`dx, dy, dz`

Explicitly set the level-set grid spacing in each direction. If set, these arguments override the automatic setting of `dx`, `dy`, and `dz`, which uses `resolution`.

`fill.buried`

For deposition, material is deposited on the surface exposed to the upper gas region. With `fill.buried` specified, deposition also occurs inside the buried gas bubbles that may exist.

`fill.buried.interface`

Specifies the material to fill gas bubbles at material interfaces. The material must already be present in the simulation.

**NOTE** This argument applies only to 3D deposition.

`fill.buried.match.surrounding`

Similar to `fill.buried`, but instead of depositing the deposition material in gas bubbles, this option fills gas bubbles that are completely surrounded by a single material with that material, removing the bubbles from the domain entirely. Gas bubbles at material interfaces remain unfilled but can be filled using `fill.buried.interface`.

**NOTE** This argument applies only to 3D deposition.

`force.analytic`

When performing isotropic etching or deposition, this argument permits the use of an analytic algorithm even when a boundary collision will occur. Otherwise, self-intersections will force the use of the level-set algorithm. For very large structures or very small etching or deposition thicknesses, the level-set algorithm may consume too much memory and time.

`force.full.levelset, force.full.levelset.depo, force.full.levelset.etch`

Defines the general level-set time-stepping algorithm as the default algorithm for both etching and deposition, or etching only, or deposition only, respectively.

`fourier.local.diffusivity`

Controls the artificial diffusion parameter. If `fourier.local.diffusivity` is specified, the solution is more accurate but the corners are less sharp. For complex Fourier rates, switch off `fourier.local.diffusivity` to enhance stability.

`full.resolution`

Usually, the full-time stepping level-set method is used in situations where more intricate boundaries will be generated. Default unit:  $\mu\text{m}$ .

The full-time stepping level-set method is needed for Fourier, crystallographic, and multimaterial etching types, and for etching with shadowing on. This argument allows a separate resolution setting for these cases. The default value is 0.025 compared to 0.1 for `resolution`.

`keep.closed.voids`

In the case of crystallographic deposition, enclosed voids may continue to grow and fill up. For efficiency, the algorithm checks for such voids only at the beginning of the deposition. Specifying this option instructs the algorithm to check for enclosed voids at each deposition time step, but at the cost of additional computational time.

`max.number.levelset.cells`

Specifies the maximum number of cells used by the level-set mesh. If this limit is exceeded, a warning message is issued. Default:  $1.0 \times 10^9$  (or  $1000 \times 1000 \times 1000$  cells).

`min.gas.thickness`

Minimum thickness of the gas layer at the top of the simulation structure. Default value and unit: 0.1  $\mu\text{m}$ .

## A: Commands

mgoals

min.levelset.size

Specifies the minimum size for the level-set mesh. Usually, the level-set mesh size scales with the operation according to the resolution factor and the etching or deposition thickness. However, for thin etching or deposition steps, this may lead to a small level-set mesh causing excessive memory use and simulation time. Often, it is not necessary (for thin layers, a mesh size between thickness/2.0 and thickness/3.0 is usually sufficient). This argument limits the mesh size and, therefore, limits computational expense. Default value and unit:  $1.0 \times 10^{-4} \mu\text{m}$ .

print.params

Prints the current MGOALS parameters.

reinitfrequency

Level-set reinitialization is performed every `reinitfrequency` time step in level-set operations. A reinitialization algorithm is run to condition the level-set distance function to reduce the effect of *contour bunching*, which can cause etching distances to be less than expected. The default value is 0, which means that no reinitialization is performed.

reinititerations

The internal reinitialization algorithm reinitializes first the 0 level set and works outwards from the front with higher numbers of iterations. Default: 1. This argument only comes into operation if `reinitfrequency` is nonzero.

remove.floating.regions

Determines whether MGOALS automatically removes regions that are not attached to the bottom of the structure. Default: true.

repair.2d, repair.2d.deposit, repair.2d.etch, repair.2d.photo  
repair.3d, repair.3d.deposit, repair.3d.etch, repair.3d.photo

Controls the default behavior of the boundary repair operation in two and three dimensions. The options also control whether repairs are enabled in etching and deposition. By default, boundary repairs are disabled in two dimensions and enabled in three dimensions.

repair.angle

Controls the dihedral angle at which repairs are performed. The algorithm attempts to repair any surface section with a dihedral angle less than `repair.angle`. Default value and unit:  $1^\circ$ .

repair.crystal.depo.facets

During crystallographic deposition, boundary conditions near neutral walls can lead to a moving front that is perpendicular to the wall, resembling a break in facets. This option

allows additional control by adding a repair step to make the surface near neutral walls more smooth.

`resolution`

Specifies the minimum number of level-set cells across the thickness of a deposited or etched layer. For example, `resolution=0.2` implies five cells. Default: 0.1.

`trapezoidal.algorithm`

Sets the algorithm used for trapezoidal etching:

- A value of 2 selects the preferred, newer algorithm, which improves the quality of produced shapes, resulting in better meshes after etching.
- A value of 1 selects the earlier algorithm.

Default: 2.

`use.brep.2d`

Switches on the brep structure mode for two dimensions when handling structural changes such as 2D etching and 2D deposition. Default: false.

The boundary representation (brep) structure mode in two dimensions handles structural changes similarly to how structural changes are handled by default in three dimensions. A brep of the structure is used and modified rather than the volume mesh.

Using brep reduces runtimes by avoiding unnecessary meshing operations and increases stability and accuracy by eliminating both boundary simplification and variable interpolation associated with remeshing between structural modification operations.

M-2016.12-SP2, M-2016.12-SP1, M-2016.12, L-2016.03-SP2, L-2016.03-SP1,  
L-2016.03, K-2015.06-SP2, K-2015.06-SP1, K-2015.06, J-2014.09-SP2,  
J-2014.09-SP1, J-2014.09, I-2013.12-SP2, I-2013.12-SP1, I-2013.12,  
H-2013.03-SP2, H-2013.03-SP1, H-2013.03, G-2012.06-SP2, G-2012.06,  
F-2011.09-SP1, F-2011.09, E-2010.12, D-2010.03

Sets the backward compatibility of parameters and algorithms to the specified version. Support is available for all the listed versions except Version D-2010.03, for which there is only partial support.

## Arguments: Deprecated

The following arguments are deprecated since they belong to the deprecated MGOALS mesh generator: `max.box.angle`, `max.lateral.size`, `max.neighbor.ratio`, `minedge`, `min.normal.size`, `normal.growth.ratio`, and `offsetting.maxlevel`.

Instead, use the equivalent Sentaurus Mesh pdb parameters (see [Table 88 on page 742](#)).

## A: Commands

mgoals

The following arguments are deprecated and have no equivalent parameters in Sentaurus Mesh:  
`maxangle`, `nlayers`, `sliver.split`, `sliver.smooth`, and `sliver.swap`.

It is suggested that you remove these arguments from command files since they may not be accepted in future releases.

### Description

This command allows you to define parameters for MGOALS-related operations.

### Examples

Explicitly set the vertical level-set mesh spacing to 0.01  $\mu\text{m}$  and the horizontal level-set mesh spacing to 0.02  $\mu\text{m}$ . Reinitialization of the level-set distance function is performed every five time steps, and every reinitialization is performed to an internal iteration accuracy of four iterations:

```
mgoals dx= 0.01 dy= 0.02 reinitfrequency= 5 reinititerations= 4
```

---

## MoleFractionFields

Returns the component fields and the field values in alloys for a given mole fraction.

### Syntax

```
MoleFractionFields <material> <xMoleFraction> [<yMoleFraction>]
```

### Arguments

<material>

Specifies an alloy material such as SiliconGermanium.

<xMoleFraction>, <yMoleFraction>

Specify the required mole fraction using a value between 0 and 1 inclusively. The second mole fraction <yMoleFraction> is needed for quaternary III–V materials.

### Description

This command provides a convenient way to initialize component fields in alloy materials. It can be used with the `fields.values` argument of the `init` and `deposit` commands, and the `epi.doping` and `epi.doping.final` arguments of the `diffuse` and `temp_ramp` commands.

### Examples

Initialize the structure and set the Germanium and Silicon fields so that the mole fraction is 0.2, that is,  $\text{Si}_{0.8}\text{Ge}_{0.2}$ :

```
init fields.values= [MoleFractionFields SiliconGermanium 0.2]
```

The output from this command is:

```
sprocess> MoleFractionFields SiliconGermanium 0.2
Silicon = 3.9067200000000015e+22 Germanium = 9.766800000000012e+21
```

Deposit  $\text{Al}_{0.2}\text{In}_{0.1}\text{Ga}_{0.7}\text{As}$ :

```
deposit AlInGaAs isotropic thickness= 0.1<um> \
fields.values= [MoleFractionFields AlInGaAs 0.2 0.1]
```

### See Also

[GetMoleFractionFields on page 967](#)

[SetMoleFractionFields on page 1182](#)

## A: Commands

optimize

---

# optimize

Optimizes the specified parameters to achieve the required target values.

## Syntax

```
optimize
  model.function=<c>
  model.parameters= {<c1> <c2> <c3> ...}
  (target= <list> | target.file=<c>)
  [history=<c>]
  [max.iter=<n>]
  [min.abs= <list>]
  [min.rel= <list>]
  [param.init= {<c1>=<n> <c2>=<n> <c3>=<n> ...}]
  [param.log= {<c1> <c2> ...}]
  [param.lower= {<c1>=<n> <c2>=<n> <c3>=<n> ...}]
  [param.upper= {<c1>=<n> <c2>=<n> <c3>=<n> ...}]
  [tolerance=<n>]
  [weight= <list>]
```

## Arguments

history

Specifies the file where the history of the optimization is stored. The history of the parameters, the corresponding target results, and the RMS errors are displayed in columns with each row corresponding to a loop.

max.iter

Specifies the maximum number of iterations allowed in the optimization loop.  
Default: 500.

min.abs

Lists the minimum absolute error for each target. If specified, the list must be the same length as the number of targets. It is the minimum target value for which the absolute error is used to calculate the target error during optimization. This value is compared with the absolute target value. The default is given by `pdbGetDouble Optimizer min.abs`, which defaults to 1.e-10 for all targets.

min.rel

Lists the minimum relative error for each target. If specified, the list must be the same length as the number of targets. It is the minimum target ratio for which the relative error is used to calculate the target error during optimization. This value is compared with the

ratio of the absolute target value to the maximum absolute target value. The default is given by `pdbGetDouble Optimizer min.rel`, which defaults to 1.e-10 for all targets.

`model.function`

Name of a user-defined Tcl procedure. The arguments of the procedure are those specified in `model.parameters` and are in the same order as in `model.parameters`. The procedure computes and returns the results of the model.

`model.parameters`

Lists the names of the parameters to be optimized.

`param.init`

Lists the initial values of the parameters to be optimized. If not specified, the default value is 0.5.

`param.log`

Lists the names of any parameter whose value you want to vary logarithmically during optimization.

`param.lower`

Lists the lower bound values of the parameters to be optimized. If not specified, the default value is 0.0.

`param.upper`

Lists the upper bound values of the parameters to be optimized. If not specified, the default value is 1.0.

`target`

Lists the required target data that the optimization will attempt to achieve by varying the values of parameters listed in `model.parameters`.

**NOTE** If you use `target` for a fitting problem, you can set up the independent variable data using a global Tcl variable and use it in your user-defined Tcl procedure specified by `model.function`.

You can specify either `target` or `target.file`, but not both.

## A: Commands

optimize

target.file

Specifies a text file (SIMS data, for example) that can be used to set target values. The file has two columns of data: The first column contains independent variable data, and the second column contains the corresponding target data. The independent variable and the target data must be in pairs. For convenience, the independent variable is saved in a global Tcl variable named opt.independent.var when loading the target file. You can use it directly in your user-defined Tcl procedure specified by model.function.

You can specify either target or target.file, but not both.

tolerance

Specifies the root-mean-square (RMS) error for convergence criterion. The optimization terminates when the RMS error of targets is smaller than tolerance. The default value is given by pdbGetDouble Optimizer Tolerance, which defaults to 0.1.

weight

Lists the weighting factors for targets. If specified, the list must be the same length as the number of targets. The weights control the importance of individual targets in calculations of the error during optimization. For a fitting problem, you do not need to specify weight because all targets have the same importance.

The default is given by pdbGetDouble Optimizer Weight, which defaults to 1.0 for all targets.

## Description

This command optimizes the specified parameters to achieve the required target values. Before using the optimize command, you must define a Tcl procedure that computes the results of the model, given a set of valid model parameters. The result of the command is a Tcl list with the optimized parameters in the format:

```
{<c1> <n> <c2> <n> ... rmsError(%) <n> TotalLoops <n>}
```

## Examples

The following example is a procedure to optimize the process conditions for the given oxide thickness:

```
fproc optFunc {temp dose}
{init tdr= init
 implant Phosphorus dose= $dose energy= 80
 diffuse temperature= $temp time= 20 O2
 set z= NetActive name= NetActive store
 set tox [interface Silicon /Oxide y=0.1]
 set lox [interface Oxide /Gas y=0.1]
 set thi [expr $tox -$lox]
```

```
        return $thi
    }
```

The `optimize` command with the above procedure would be:

```
optimize model.function= optFunc model.parameters= {temp dose} \
param.init= {temp=1000 dose=1E14} \
param.lower= {temp=900 dose=1E12} \
param.upper= {temp=1200 dose=1E15} \
param.log= {dose} \
target= {0.06} \
max.iter= 500 \
tolerance= 0.1 \
min.abs= {1.e-10} \
min.rel= {1.e-10} \
history= test.dat
```

The following example is a procedure for a fitting problem. The global Tcl variable `opt.independent.var` was set to store the independent variable data after the input target file is loaded. You can use it directly in the user-defined Tcl procedure:

```
fproc optFunc {cja vja mja} {
    global {opt.independent.var}
    foreach value ${opt.independent.var} {
        lappend z [expr $cja/(1+$value/$vja)**$mja]
    }
    return $z
}
```

The `optimize` command with the above procedure would be:

```
optimize model.function= optFunc model.parameters= {cja vja mja} \
param.init= {cja=0.2 vja=5. mja=0.5} \
param.lower= {cja=0.1 vja=2. mja=0.1} \
param.upper= {cja=0.4 vja=7. mja=0.9} \
target.file= model.dat \
max.iter= 500 \
tolerance= 0.1 \
history= test.dat
```

## A: Commands

paste

---

# paste

Assembles 2D or 3D simulations by incorporating fragments from a TDR file.

## Syntax

```
paste
  tdr=<c>
  direction= "left" | "right" | "front" | "back"
  [Adaptive]
```

## Arguments

Adaptive

If specified, Adaptive switches on adaptive meshing. Parameters for adaptive meshing are described in [Adaptive Mesh Refinement on page 729](#). The default is the return value of `pdbGet Grid Adaptive`.

direction

Selects the side where to paste the incoming simulation. In three dimensions, the new structure can be pasted on the left, right, front, or back side. In two dimensions, only the left or right sides are used.

tdr

Name of the file to be imported and pasted into the current simulation.

## Description

This command reads a TDR file containing valid geometry and appends it (pastes it) to the current structure. The new structure is displaced automatically by the correct amount to properly fit at the specified side, but the structures are not stretched automatically. If the dimensions of nongas materials at the pasting sides are not the same, the command fails and quits.

The dimension of all parts must match: You cannot mix two and three dimensions. In addition, in two dimensions, only the `direction` values "left" and "right" are supported.

The `paste` command allows for the assembly of complex 2D or 3D structures by reading the different pieces from TDR files and putting all of them together.

## Examples

Append the structure from the file `propertyx_fps.tdr` to the right side (maximum y-coordinate) of the current structure:

```
paste tdr= "propertyx" direction= "right"
```

## See Also

[Inserting Polygons on page 825](#)

[struct on page 1217](#)

## pdbDelayDouble

Retrieves an expression for a double parameter that will be evaluated at each time step during diffusion.

### Syntax

```
pdbDelayDouble <c> <c> ...
```

### Arguments

<c>

This argument can be any double parameter declared in the parameter database and any double parameter declared by the user in user-defined models. In all cases, the argument must be specified with the full hierarchical path for the double parameter.

### Description

This command is typically called from Alagator to retrieve a parameter expression. Since among other things, the temperature can change during a diffusion step, the evaluation of Arrhenius expressions must be delayed until the temperature is known. This command provides this functionality.

### Examples

Return an expression for D0 (not a value):

```
pdbDelayDouble Si B D0
```

---

## **pdbsdiff**

Compares the current structure with one from a TDR file.

### **Syntax**

```
pdbsdiff <c> <c>
```

### **Arguments**

<c>

Specifies the full path or prefix of the TDR files to be compared. The prefix is the file name without \_fps.tdr.

### **Description**

The command reports any differences between the parameters stored and any differences in value.

### **Examples**

Compare the pdbs differences between n1\_fps.tdr and n2\_fps.tdr:

```
pdbsdiff n1 n2
```

## **pdbDopantLike**

Creates new dopants in materials.

### **Syntax**

```
pdbDopantLike <c> <c>
```

### **Arguments**

<c>

The first argument must be the name of the material.

The second argument must be the name of the new dopant.

### **Description**

If dopants are not present in a material, an error message is displayed.

### **Examples**

Create a new dopant called MyDopant in silicon. You can select dopant-related diffusion switches (such as DiffModel and ActiveModel) for MyDopant:

```
pdbDopantLike Silicon MyDopant
```

---

## pdbExprDouble

Retrieves an expression for a double parameter without evaluating.

### Syntax

```
pdbExprDouble <c> <c> ...
```

### Arguments

<c>

This argument can be any double parameter declared in the parameter database and any double parameter declared by the user in user-defined models. In all cases, the argument must be specified with the full hierarchical path for the double parameter.

### Description

This command is typically called from Alagator to retrieve a parameter expression. If the parameter depends on solution names, data fields, and so on, the evaluation of the expression must be delayed until the solution time. This command provides this functionality.

### Examples

Return an expression for Bulk (not a value):

```
pdbExprDouble Si Mechanics BulkModulus
```

## A: Commands

### pdbGet and Related Commands

---

## pdbGet and Related Commands

All these commands retrieve database parameters:

- pdbGet
- pdbGetArray
- pdbGetBoolean
- pdbGetDouble
- pdbDelayDouble
- pdbGetDoubleArray
- pdbGetElement
- pdbGetFunction
- pdbGetString
- pdbGetSwitch
- pdbGetSwitchString

Only pdbGet has syntax checking.

### Syntax

```
pdbGet <c> <c> ...
```

### Arguments

<c>

This argument can be any double parameter declared in the parameter database and any double parameter declared by the user in user-defined models. In all cases, the argument must be specified with the full hierarchical path for the double parameter.

### Description

These commands are used to obtain parameters that reside in the property database, which is hierarchical and is indicated by passing a series of strings to the command. In the command file, the command pdbGet must replace all other pdbGet\* commands because the type of the parameter and the syntax are checked automatically.

If a parameter does not exist in the directory, the tool exits and prints a list of parameters that can be found. Normal aliasing is applied to each string before the parameter is retrieved from the database.

The following commands all return 0 if the parameter is not found:

- `pdbGetArray`
- `pdbGetBoolean`
- `pdbGetDouble`
- `pdbDelayDouble`
- `pdbGetDoubleArray`
- `pdbGetElement`
- `pdbGetFunction`
- `pdbGetString`
- `pdbGetSwitch`

The command `pdbGetSwitchString` returns nothing if the parameter is not found.

These commands have a slight performance advantage and will not exit if a parameter has not been defined, so they are preferred for Aligator scripting.

The command `pdbGetSwitch` returns an integer value of a switch, and the command `pdbGetSwitchString` returns the string value. For example, if a switch has the choices a, b, or c, and a is chosen, `pdbGetSwitch` returns 0, and `pdbGetSwitchString` returns a.

## Examples

Retrieve the current value of `StressHistory`. The parameter `StressHistory` is known, but if it is spelled incorrectly, Sentaurus Process exits and prints a list of known parameters at the `Mechanics` level:

```
pdbGet Mechanics StressHistory
```

Retrieve `StressHistory` without syntax-checking. The command returns 0 if not found. Sentaurus Process exits if there is a type mismatch between `StressHistory` and `Boolean` (which is not the case in this example):

```
pdbGetBoolean Mechanics StressHistory
```

**A: Commands**

`pdbsAvailable`

---

## **pdbsAvailable**

Checks whether the given pdb command is available.

### **Syntax**

```
pdbsAvailable <c> <c> ...
```

### **Arguments**

<c>

Specifies the pdb command.

### **Description**

If the pdb command exists, the pdbsAvailable command returns 1; otherwise, it returns 0.

### **Examples**

Return 1 if the command "Silicon MyData" is available:

```
pdbsAvailable Silicon MyData
```

## **pdbLike**

Creates a new pdb parameter like an existing parameter in a material.

### **Syntax**

```
pdbLike <c> <c> <c>
```

### **Arguments**

<c>

The first argument must be the name of the material.

The second argument must be the name of the new pdb parameter.

The third argument must be the name of an existing pdb parameter.

### **Description**

This command is used to create a new node in the parameter database where the sub-parameters of this node are inherited from an existing node in the database. It is typically used when creating a new solution variable to inherit parameters from an existing solution variable.

### **Examples**

Create a new parameter called MyBoron in silicon:

```
pdbLike Silicon MyBoron Boron
```

MyBoron inherits all the parameters defined for Boron in silicon including the user-defined ones. If MyBoron was defined as a solution name, all the inherited callback procedure names and parameters will be used to build the diffusion equations. This is a fast way of introducing a new dopant that is like an existing one.

### **See Also**

[solution on page 1203](#)

## A: Commands

### pdbSet and Related Commands

---

## pdbSet and Related Commands

All of the following commands set database parameters:

- pdbSet
- pdbSetArray
- pdbSetBoolean
- pdbSetDouble
- pdbSetDoubleArray
- pdbSetElement
- pdbSetFunction
- pdbSetString
- pdbSetSwitch

Only pdbSet has syntax checking.

### Syntax

```
pdbSet <c> <c> ... <value>
```

### Arguments

<c>

This argument can be any parameter declared in the parameter database and any parameter declared by users in user-defined models. In all cases, the argument must be specified with the full hierarchical path for the parameter.

<value>

The value associated with the type of the parameter. For example, a double value must be given for a Double parameter type.

### Description

These commands are used to set parameters that reside in the property database, which is hierarchical and is indicated by passing a series of strings to the command. In the command file, the command pdbSet must replace all other pdbSet\* commands because the type of the parameter and the syntax are checked automatically. If a parameter does not exist in the directory, the tool exits and prints a list of parameters that can be found. Normal aliasing is applied to each string before the parameter is retrieved from the database for all these commands.

The following commands all create a new parameter if one does not already exist:

- `pdbSetArray`
- `pdbSetBoolean`
- `pdbSetDouble`
- `pdbSetDoubleArray`
- `pdbSetFunction`
- `pdbSetString`

These commands have a slight performance advantage, and Sentaurus Process does not exit if a parameter has not been defined, so they are preferred for Aligator scripting. The property database uses the CGS system of units, except for activation energies [eV].

The command `pdbSet` checks the type of variable trying to be set and checks that type against the `<value>` passed. The command `pdbSetDouble` takes a double for a value and, similarly, `pdbSetString` takes a string and `pdbSetBoolean` takes a Boolean (1 or 0). The command `pdbSetSwitch` will set a value for existing switches. If a switch is not found, a new one will be created.

The command `pdbSetArray` defines the array for string data.

The data type `DoubleArray` has a special format and can be modified in several different ways depending on the changes required.

This type is usually used for charge state-dependent parameters, in which case, the array index refers to the charge state. For example, the database entry for `Silicon Interstitial ChargeStates` is a list of length 10; the first entry is -2, the second entry is 0 (which means `ChargeStates[-2]=0`), the third entry is -1, and the fourth is `{[Arrhenius 5.68 0.48]}`, which means `ChargeStates[-1]=[Arrhenius 5.68 0.48]` and so on.

There are also arrays that are intended for double sums. In this case, the array index entries have a comma-separated field. For example, with `Silicon Boron Interstitial kfKickOut`, the first entry (which corresponds to an array index) is `{-2, -2}`. The following examples show how to set and change these types.

The command `pdbSetElement` modifies the value of one element in an array.

**NOTE** The arguments for `pdbSetDouble`, `pdbSetDoubleArray`, and `pdbSetBoolean` must evaluate to numeric data. Calls to procedures or to the `pdbDelayDouble` command in the arguments may cause errors if they are not constructed correctly.

## A: Commands

### pdbSet and Related Commands

## Examples

Set the Dstar parameter for boron in silicon; exit with list if not found:

```
pdbSet Si B Dstar 1e-7
```

Set index 0 of ChargeStates to 0.1:

```
pdbSet Si Int ChargeStates 0 0.1
```

Set all members of ChargeStates (index 0 = 0.1, and so on):

```
pdbSet Si Int ChargeStates {0 0.1 1 0.2 3 0.3}
```

Set one index of a double array meant for double charge state indexing:

```
pdbSet Si B Int KfKickOut -2,1 {[expr 4.0*3.14159*([Arrhenius 0.1 0.2]+[Arrhenius 0.3 0.4])]}
```

Now for the non-syntax-checked versions:

Set Dstar; create Dstar if it does not already exist (in this example, Dstar would exist):

```
pdbSetDouble Si B Dstar 1e-7
```

Set the DiffModel in silicon to Pair:

```
pdbSetSwitch Si Dopant DiffModel Pair
```

Create a new DoubleArray, index 0 = 0.1, and so on:

```
pdbSetDoubleArray Si MyVar MyArray {0 0.1 1 0.2 3 0.3}
pdbSetArray MyArray {0 abc 1 def 2 ghi}
pdbGetArray MyArray ;# print "0 abc 1 def 2 ghi"
pdbGetElement MyArray 1 ;# print "def"
pdbSetElement MyArray 1 jkl ;# modifies A[1] data from "def" to "jkl"
```

---

## pdbUnSet-Related Commands

All these commands unset database parameters:

- pdbUnSetBoolean
- pdbUnSetDouble
- pdbUnSetDoubleArray
- pdbUnSetString

### Syntax

```
pdbUnSetBoolean <c> <c> ...
pdbUnSetDouble <c> <c> ...
pdbUnSetDoubleArray <c> <c> ...
pdbUnSetString <c> <c> ...
```

### Arguments

<c>

This argument can be any parameter declared in the parameter database and any parameter declared by users in user-defined models. In all cases, the argument must be specified with the full hierarchical path for the parameter.

### Description

This command temporarily removes parameters from the parameter database during the simulation.

### Examples

Remove the Derived.Materials list of InGaAs material:

```
pdbUnSetString InGaAs Derived.Materials
```

## PDE2KMC

Translates and transfers Sentaurus Process fields to Sentaurus Process KMC.

### Syntax

PDE2KMC

### Description

This command is called automatically when a switch from the PDE solver to the Sentaurus Process KMC solver is detected. It translates the continuum concentrations into suitable particle distributions to be used by Sentaurus Process KMC.

The atomization is performed using the `select` command with the appropriate KMC species names.

The translation between PDE fields and KMC species is performed with a mapping that translates the field names into their atomistic counterparts. This translation is made as accurately as possible, but sometimes a perfect one-to-one mapping is not possible. In that case, meaningful approximations are used. For example, `ICluster` is translated into `I4`.

A complete list of these translations is available in the `KMC.tcl` file.

### See Also

[SetAtomistic on page 1175](#)

---

## photo

Creates a photoresist layer of the specified thickness outside the mask.

### Syntax

```
photo
[Adaptive] [mask=<c>] [repair] [sde= {<c>}]
[thickness=<n>] [<m>|<cm>|<um>|<nm>]
```

### Arguments

#### Adaptive

If specified, Adaptive switches on adaptive meshing. Parameters for adaptive meshing are described in [Adaptive Mesh Refinement on page 729](#). The default is the return value of `pdbGet Grid Adaptive`.

#### mask

Name of the mask to be used to create the photoresist. The photoresist is deposited in the openings of the mask.

#### repair

In 3D MGOALS mode, small regions are removed automatically by default. Sometimes, this causes small gas bubbles in the structure or other problems. Use `!repair` to switch off the small region removal.

#### sde

String used to specify parameters and algorithms for 3D simulations using Sentaurus Structure Editor. By default, `mask` and `thickness` are translated into appropriate Sentaurus Structure Editor commands. If an algorithm is specified using `sde`, it overwrites the algorithm used by default for isotropic or anisotropic etching, for example:

```
photo thickness= 2<um> mask= mask1 sde= {"algorithm" "lopx"}
```

#### thickness

Specifies the thickness of the photoresist. Default value and unit:  $2.0\text{ }\mu\text{m}$ .

### Description

The mask must have been defined using a `mask` command. If the photoresist must be deposited inside of the mask, the `negative` argument must be defined in the `mask` command.

## A: Commands

photo

### Examples

Create a resist layer of 1  $\mu\text{m}$  thickness. The resist layer material will appear in open areas of the mask `mask1`, that is, it will be the negative of `mask1`:

```
photo thickness= 1<um> mask= mask1
```

Create a resist layer of 2  $\mu\text{m}$  thickness. The resist layer will have the same polarity as `mask2`:

```
photo mask= mask2
```

### See Also

[mask on page 1065](#)

---

## plot.1d

Plots a 1D cross section.

### Syntax

```
plot.1d
  [boundary] [clear] [close] [color=<c>] [fix.ratio] [label=<c>]
  [max= <list>] [min= <list>]
  [name=<c>] [rescale] [symb=<c>] [title=<c>]
  [x=<n>] [<m>|<cm>|<um>|<nm>]
  [y=<n>] [<m>|<cm>|<um>|<nm>]
  [z=<n>] [<m>|<cm>|<um>|<nm>]
```

### Arguments

**boundary**

Specifies that any material boundaries that are crossed must be drawn in as vertical lines on the plot. Default: false.

**clear**

Specifies whether the graphics screen must be cleared before the graph is drawn. Default: true (the screen is cleared).

**close**

Closes the plot window.

**color**

Specifies the line color for the plot. It can be any color supported by X11 hardware and named in the color database.

**fix.ratio**

Specifies the x-, y-axis ratio to be fixed. Default: false.

**label**

Specifies the name of the line in the legend of the plot window. The default is the name of the current dataset.

## A: Commands

### plot.1d

max

List of numeric values that will be the ends of the x- and y-axis. The first argument is the x-value and the second is the y-value. A single value is always interpreted as the x-value. The default is the maximum extent of the current structure.

min

List of numeric values that will be the ends of the x- and y-axis. The first argument is the x-value and the second is the y-value. A single value is always interpreted as the x-value. The default is the minimum extent of the current structure.

name

Name of a data field. This allows plots to be created without using the `select` command.  
Default: `z_Plot_Var`.

rescale

Rescales the plot to fit the entire simulation domain.

symbol

Specifies a symbol type to be drawn on the cross-sectional line. Each point is drawn with the specified symbol. It defaults to no symbol. Whatever character is entered is placed at each data point on the plot.

title

Specifies the title of the plot window.

x, y, z

Specify the constant values of a line along which sectioning is performed. In one dimension, these arguments are not necessary. In two dimensions, only one of x or y can be specified for a given device. Specifying x produces a horizontal slice through the device and y specifies a vertical slice. An easy way to remember is that the cross section is taken at the constant value specified. For a 3D simulation, two of these three values must be specified. Default unit:  $\mu\text{m}$ .

## Description

This command plots cross sections vertically or horizontally through the device with arguments to provide for initialization of the graphics device and plotting of axes. This command can optionally draw vertical lines whenever a material boundary is crossed.

## Examples

Clear the screen, draw a set of axes, and draw the data along a horizontal cross section at  $x = 1.0 \mu\text{m}$ . Each point is drawn with symbol 1:

```
plot.1d x= 1.0 symb= 1 clear
```

Draw a horizontal cross section at  $x = 2.0 \mu\text{m}$  on the previous set of axis. The line is labeled Lateral in the legend:

```
plot.1d x= 2.0 clear label= Lateral
```

## See Also

[select on page 1168](#)  
[slice on page 1199](#)

**A: Commands**plot.2d

---

## plot.2d

Plots a 2D xy graphic.

### Syntax

```
plot.2d
  [boundary] [clear] [close] [col.bound=<c>] [col.grid=<c>]
  [edges] [faces] [fill] [fix.ratio] [gas] [grid] [kmc] [label.bound]
  [max= <list>] [min= <list>]
  [nodes] [rescale] [title=<c>]
  [vector=<c>]
  [vlength=<n>] [<m>|<cm>|<um>|<nm>]
  [vmax=<n>] [<m>|<cm>|<um>|<nm>]
  [x=<n> | y=<n> | z=<n>] [<m>|<cm>|<um>|<nm>]
```

### Arguments

**boundary**

Specifies that the device outline and material interfaces must be drawn. Default: false.

**clear**

Specifies that the graphics screen must be cleared before the graph is drawn. Default: true (the screen is cleared).

**close**

Closes the plot window.

**col.bound**

Specifies the color of the boundary. Any valid X11 color can be specified.

**col.grid**

Specifies the color of the grid. Any valid X11 color can be specified.

**edges**

Prints the edge indices on the plot. Default: false.

**faces**

Prints the face indices on the plot. Default: false.

`fill`

Specifies that the device must be drawn with the proper aspect ratio. If `fill` is false, the device is drawn with the proper aspect ratio. If `fill` is true, the device is expanded to fill the screen. Default: false.

`fix.ratio`

By default, the x to y ratio is now fixed. This can be switched off using `!fix.ratio`.

`gas`

Specifies that the grid in the gas must also be plotted. Default: false (no gas grid is shown).

`grid`

Specifies that the numeric grid on which the problem was solved must be drawn. Default: false.

`kmc`

Plots particles in an atomistic KMC simulations as dots.

`label.bound`

Name of the material in the lower-left corner of the material region.

`max`

List of numeric values that will be the ends of the x- and y-axis, respectively. The first argument is the x-value and the second is the y-value. A single value is always interpreted as the x-value. The default is the maximum extent of the current structure. Default unit:  $\mu\text{m}$ .

`min`

List of numeric values that will be the ends of the x- and y-axis, respectively. The first argument is the x-value and the second is the y-value. A single value is always interpreted as the x-value. The default is the minimum extent of the current structure. Default unit:  $\mu\text{m}$ .

`nodes`

Prints the node indices on the plot. Default: false.

`rescale`

Rescales the plot to fit the whole simulation domain.

## A: Commands

### plot.2d

**title**

Specifies the title of the plot window.

**vector**

Name of a vector field. This indicates arrows proportional to the size of the vector and in the direction of the vector at each node. This argument does not work in 3D simulations.

**vlength**

Scales the length of the vectors so that the maximum vector has length **vlength**. Default value and unit: 0.1  $\mu\text{m}$ .

**vmax**

Use this as the maximum velocity instead of searching for it. Default unit:  $\mu\text{m}$ .

**x, y, z**

For 2D simulations, these arguments are unnecessary. In three dimensions, one of these three must be specified to indicate the cutline through the structure. Default unit:  $\mu\text{m}$ .

## Description

Usually, this command is used to look at material boundaries and grids; however, it also can be used to plot a flow field. This command can be executed immediately before a `contour` command to allow isoconcentration lines to be plotted in context with the structure.

To obtain standard color and other settings for the `plot.2d` window, use the following command from the command line:

```
unix:> xrdb -merge ${STROOT}/tcad/${STRELEASE}/lib/score/XFloops
```

## Examples

Draw the triangular grid and axis. Each material is plotted in a different color:

```
plot.2d grid
```

Draw the material interfaces with the minimum x- and y-values of 2.0  $\mu\text{m}$  and 5.0  $\mu\text{m}$ :

```
plot.2d boundary min= {2 5}
```

Draw the material interfaces and place symbols at each coordinate in the mesh:

```
plot.2d boundary diamonds
```

Plot the Velocity vector field. The maximum arrow drawn will have a length of 0.1  $\mu\text{m}$ . The plot surface will not be cleared:

```
plot.2d vector= Velocity vlength= 0.1 !clear
```

## See Also

[bound on page 911](#)  
[Compatibility on page 915](#)  
[contour on page 921](#)  
[select on page 1168](#)  
[slice on page 1199](#)

## A: Commands

plot.xy

---

# plot.xy

Prepares an xy plot to draw on.

## Syntax

```
plot.xy  
  [clear]  
  [max= <list>] [min= <list>]  
  [x.axis=<c>] [y.axis=<c>] [x.log] [y.log]
```

## Arguments

clear

Clears the existing plot surface. Default: true.

max

List of numeric values that will be the ends of the x- and y-axis, respectively. The first argument is the x-value and the second is the y-value. A single value is always interpreted as the x-value. The default is the maximum extent of the current structure.

min

List of numeric values that will be the ends of the x- and y-axis, respectively. The first argument is the x-value and the second is the y-value. A single value is always interpreted as the x-value. The default is the minimum extent of the current structure.

x.axis, y.axis

Specify the labels for the x-axis and y-axis.

x.log, y.log

Specify whether there is a linear or log axis. If x.log or y.log is selected, the logarithm of the values on the point.xy command are taken. The axis also will have log scale form.

## Description

This command configures a 2D plot surface for use with the point.xy command. This prepares the axis scaling and labels, and controls the log axes.

Using this command and the point.xy command could simulate all other commands in this section.

## Examples

Prepare a plot area:

```
plot.xy min= {1 0.0} max= {3600 0.75} x.axis= Time y.axis= Thickness
```

## See Also

[point.xy on page 1122](#)

[select on page 1168](#)

## A: Commands

point

---

# point

Creates a point, for example, for a mask polygon.

## Syntax

```
point
  [clear]
  [coord= {
    <n> [<m> | <cm> | <um> | <nm>]
    <n> [<m> | <cm> | <um> | <nm>]
    <n> [<m> | <cm> | <um> | <nm> ] }
  [list] [name=<c>]
```

## Arguments

clear

Clears the list of all points. If name is specified, it clears only this point information.

coord

Defines the coordinates of the point. For a 3D point, all three coordinates must be specified.  
If only two are defined, a 2D layout point in the yz plane is assumed. Default unit:  $\mu\text{m}$ .

list

Returns the list of currently defined points. If name is given, it prints the information for this point only.

name

Name of the point.

## Description

This command defines a point in three dimensions or a 2D point in the yz plane. It can be used to construct polygons to define masks.

## Examples

Define a 2D point with the coordinates  $y = 0$  and  $z = -1.5$ :

```
point name= p1 coord= {0 -1.5}
```

Print the list of defined points:

```
LogFile [point list]
```

**See Also**

[mask on page 1065](#)

[polygon on page 1124](#)

**A: Commands**point.xy

---

## point.xy

Adds a line segment to a plot.

### Syntax

```
point.xy  
  x=<n>  y=<n>  
  [color=<c>]  [move]  [name=<c>]  [symb=<c>]
```

### Arguments

color

Specifies the color for the line. It can be any color supported by X11 hardware and named in the color database.

move

Instead of drawing from the last point, the graphics pen is placed at this point without moving. Using move with symb draws scatter plots.

name

Name of a line, so that points can be added to the line at a later time. The name can be any valid character string and is used in the plot legend. If the named line does not exist, it is created.

symb

The first character of this string is used to mark the line. If no symbol is specified, none will be used. If a symbol is specified once for a line, it is used for all lines. Default: x.

x, y

Specify the values to be added to the plot.

### Description

This command adds segments to a specified line on a plot surface using X-windows-based plotting (plot.1d or plot.2d). The command is used to plot calculated values, data, or direct outputs from the simulation. The values can be added to any named line.

## Examples

Add x- and y-values to the line named Thickness:

```
point.xy x= 60.0 y= 0.1 name= Thickness
```

## See Also

[interface on page 1030](#)  
[interpolate on page 1033](#)  
[plot.xy on page 1118](#)  
[select on page 1168](#)

## A: Commands

polygon

---

# polygon

Creates a polygon, for example, for a mask.

## Syntax

```
polygon
  clear |
  list |
  (name=<c>
    [external.sde] |
    [tdr=<c>] [materials= {<mat1> ... matn}] |
    [max= {
      <y>[<m>|<cm>|<um>|<nm>]
      <z>[<m>|<cm>|<um>|<nm>] }]
    [min= {
      <y>[<m>|<cm>|<um>|<nm>]
      <z>[<m>|<cm>|<um>|<nm>] }]
    [rectangle] |
    [points= {<point1> <point2> ... <pointn>}] [rectangle] |
    [tdr=<c>] [regions= {<reg1> ... <regn>}] |
    [segments= {
      <y_1>[<m>|<cm>|<um>|<nm>]
      <z_1>[<m>|<cm>|<um>|<nm>]
      <y_2>[<m>|<cm>|<um>|<nm>]
      <z_2>[<m>|<cm>|<um>|<nm>]
      ...
      <y_n>[<m>|<cm>|<um>|<nm>]
      <z_n>[<m>|<cm>|<um>|<nm>] }]
    }
  [xy]
```

## Arguments

clear

Clears the list of all polygons. If name is specified, it clears only the named polygon.

external.sde

Creates a polygon from an external Sentaurus Structure Editor structure (see [Sentaurus Structure Editor Interface on page 829](#)).

list

Returns a list of all polygons. If name is given, it returns the information for this polygon only.

**materials**

Specifies a material or list of materials that will be read when using `tdr`.

**max**

Maximum point for a rectangular box. It must be used with `rectangle` to create a rectangular polygon. The default is the structure bounding box maximum. Default unit:  $\mu\text{m}$ .

**min**

Minimum point for a rectangular box. It must be used with `rectangle` to create a rectangular polygon. The default is the structure bounding box minimum. Default unit:  $\mu\text{m}$ .

**name**

Name of the polygon.

**points**

Lists the point names used to specify the polygon. A minimum of three must be specified. The points must have been specified using the `point` command. The polygon is closed implicitly by connecting the first and last points.

`points` also can be used with `rectangle` to specify a rectangular polygon. In this case, two points must be given: the minimum and maximum points of the rectangle.

**rectangle**

Must be specified with `max` and `min` to define a rectangular box. Alternatively, two named points can be given (using `points`) corresponding to the minimum and maximum of the rectangle.

**regions**

Specifies a region or list of regions to be used when reading the polygon when using `tdr`.

**segments**

Lists the line segments in the  $yz$  plane (or the  $xy$  plane when  $xy$  is specified) used to specify a polygon in three dimensions. The polygon is closed implicitly by connecting the first and last points. A minimum of three segments must be given. Default unit:  $\mu\text{m}$ .

**tdr**

Name of the file from which to read the polygon. If you use `tdr`, you must specify `xy`. It allows you to use materials and regions to further specify which polygon to be read from the TDR file.

## A: Commands

polygon

xy

Defines the polygon in the xy plane instead of the default yz plane. When using `xy`, the segments are defined as  $\{x_1\ y_1\ \dots\ x_n\ y_n\}$ , and `min` and `max` as `x` `y`. You must use `xy` when specifying `tdr`. Specifying `xy` typically means that the polygon will be used for insertion rather than for masking.

### Description

This command defines a mask or uses the polygon during an insertion. One of the following must be used to create a polygon:

- `points`
- `rectangle`
- `segments`
- `tdr`

If named points are not given explicitly when forming polygons, they are generated automatically during the creation of the polygon.

### Examples

Create three identical rectangles using points and coordinates:

```
point name= p1 coord= {0.0 0.0}
point name= p2 coord= {0.0 -0.5}
point name= p3 coord= {0.5 -0.5}
point name= p4 coord= {0.5 0.0}

polygon name= Box1 points= {p1 p2 p3 p4}
polygon name= Box2 points= {p2 p4} rectangle
polygon name= Box3 min= {0.0 -0.5} max= {0.5 0.0} rectangle
```

Define an L-shaped polygon using 1D line segments:

```
polygon name= LShape \
    segments= {0.0 -1.5 0.0 -0.5 0.5 -0.5 0.5 1.5 1.5 1.5 1.5 -1.5}
```

Read the aluminum material structure in the file `points_bnd.tdr` as a polygon called `box`:

```
polygon name= "box" xy tdr= "points_bnd.tdr" materials= "Aluminum"
```

Print the list of polygons that have been defined:

```
LogFile [polygon list]
```

Delete `Box3`:

```
polygon name= Box3 clear
```

## See Also

[Inserting Polygons on page 825](#)

[insert on page 1024](#)

[mask on page 1065](#)

[point on page 1120](#)

## A: Commands

polyhedron

---

# polyhedron

Creates and stores 3D polyhedra, for later insertion with the `insert` command or for use with the `profile` command.

## Syntax

```
polyhedron
  clear |
  list |
  (
    name=<c>
    (
      brick= {
        <minx>[<m>|<cm>|<um>|<nm>]
        <miny>[<m>|<cm>|<um>|<nm>]
        <minz>[<m>|<cm>|<um>|<nm>]
        <maxx>[<m>|<cm>|<um>|<nm>]
        <maxy>[<m>|<cm>|<um>|<nm>]
        <maxz>[<m>|<cm>|<um>|<nm>] } |
        original.polyhedron=<c> |
        (polygons= <list> |
          min=<n>[<m>|<cm>|<um>|<nm>]
          max=<n>[<m>|<cm>|<um>|<nm>]) |
          (tdr=<c> [materials= <list>] | [regions= <list>])
      )
      [bbox | bbox.cm | bbox.um]
      [external.sde]
      [offset= {<x> <y> <z>}]
      ([rotate.angles= {<psi> <theta> <phi>}] [rotate.center= {<x> <y> <z>}])
      ([scale=<n>] [scale.center= {<x> <y> <z>}])
      ([stretch] [direction= x | -x | y | -y | z | -z] [length=<n>]
       [location=<n>])
    )
  )
```

## Arguments

`bbox`, `bbox.cm`, `bbox.um`

If `bbox` is specified, the `polyhedron` command returns the maximum extents of the named polyhedron in two points. If `bbox.cm` is specified, the command returns the maximum extents of the polyhedron in centimeter. If `bbox.um` is specified, the command returns the maximum extents of the polyhedron in micrometer.

**brick**

Creates a rectangular prism, given its two corners as <minx> <miny> <minz> and <maxx> <maxy> <maxz>. Default unit:  $\mu\text{m}$ .

**clear**

Removes all the previously defined polyhedra from memory.

**external.sde**

Creates a polyhedron from an external Sentaurus Structure Editor structure (see [Sentaurus Structure Editor Interface on page 829](#)).

**list**

Lists the currently defined polyhedra.

**materials**

It is used only with `tdr` and lists the materials to be included in the file. In addition to explicit material names, `bulk.materials` is available to specify all nongas materials.

**max**

Maximum x-coordinate for extrusion (see `polygons`). Default unit:  $\mu\text{m}$ .

**min**

Minimum x-coordinate for extrusion (see `polygons`). Default unit:  $\mu\text{m}$ .

**name**

Name of the polyhedron to be created.

**offset**

Specifies the offset to be applied before saving the named polyhedron.

**original.polyhedron**

Creates a new polyhedron from the specified original polyhedron before applying the transformation.

**polygons**

This argument can be used in two contexts:

- When specifying a list of polygons that form a polyhedron, it builds such a polyhedron.

## A: Commands

### polyhedron

- When specifying one planar axis-oriented polyhedron, it extrudes (using `min` and `max`) that polygon in the x-direction to form a polyhedron.

`regions`

It is used only with `tdr` and lists which regions of the TDR boundary file are included.

`rotate.angles`, `rotate.center`

By default, the location of the rotation center is the geometric center of the polyhedron, which is  $\{(\text{xmin}+\text{xmax})/2 \ (\text{ymin}+\text{ymax})/2.0 \ (\text{zmin}+\text{zmax})/2.0\}$ . The minimum and maximum coordinates of the polyhedron can be found using the `bbox` option. You can redefine the rotation center using the `rotate.center` argument.

The rotation uses the so-called intrinsic rotation of the Tait–Bryan angles, where `<psi>`, `<theta>`, and `<phi>` are angles rotated around the x-, y'-, and z"-axis, respectively. For more information, go to [https://en.wikipedia.org/wiki/Euler\\_angles](https://en.wikipedia.org/wiki/Euler_angles).

`scale`, `scale.center`

If `scale` is specified, the polyhedron is enlarged or reduced proportionally. By default, the scale center is the geometric center of the polyhedron, but you can redefine the scale center using the `scale.center` argument.

`stretch`, `direction`, `length`, `location`

If the `stretch` option is specified, the polyhedron is stretched a specified length, along the specified direction, at the specified location. By default, `direction=x`, `length=0`, and `location=0`.

`tdr`

Name of the TDR boundary file from which to read all the polyhedra.

## Description

This command creates a polyhedron and stores it under the name specified. Different mechanisms can be used to create the polyhedron. It can be read from an existing polyhedron or from a TDR boundary file; it can be defined as a brick or defined from the beginning using polygonal faces; it can be created as an extruded polygon. In addition, several transformations can be applied to the polyhedron, such as offset, rotate, scale, and stretch. When a polyhedron is defined, it can be used to perform polyhedron insertion using the `insert` command, or it can be used as a geometric parameter in the `polyhedron` argument of the `profile` command.

**NOTE** If a polyhedron is created from a TDR file (`tdr=<c>`) and is intended for use in the `profile` command, you must specify either the `materials` or `regions` argument. If no materials or regions are specified, `materials=bulk.materials` is required.

**NOTE** The final result depends on the order of the transformations, if any. If `offset`, `rotate`, `scale`, and `stretch` are all specified in the same command, Sentaurus Process executes the transformations in the following sequence starting with `offset`, then `rotate`, `scale`, and finally `stretch`.

## Examples

Load the polyhedra containing silicon and gas from the boundary file `sphere_bnd.tdr` with the name `sphere`:

```
polyhedron name= sphere tdr= sphere_bnd.tdr materials= {Silicon Gas}
```

Create a polyhedron named `prism` and extrude from  $x = -6 \mu\text{m}$  to  $x = 2 \mu\text{m}$  an already existing polygon called `triangle`:

```
polyhedron name= prism polygons= {triangle} min= -6 max= 2
```

Using the polygons `face1`, `face2`, `face3`, and `face4` (they must be correctly defined), build a polyhedron called `tetrahedron`:

```
polyhedron name= tetrahedron polygons= {face1 face2 face3 face4}
```

Define a rectangular prism (brick shape) called `smallPrism` by using its two corners, that is,  $\langle \text{minx} \rangle = -6 \mu\text{m}$ ,  $\langle \text{miny} \rangle = -4 \mu\text{m}$ ,  $\langle \text{minz} \rangle = -2 \mu\text{m}$ ,  $\langle \text{maxx} \rangle = -1 \mu\text{m}$ ,  $\langle \text{maxy} \rangle = 4.5 \mu\text{m}$ ,  $\langle \text{maxz} \rangle = 1 \mu\text{m}$ :

```
polyhedron name= smallPrism brick= {-6 -4 -2 -1 4.5 1}
```

Stretch and scale a prism:

```
polyhedron name=new_prism original.polyhedron=prism scale=2 stretch \
length= 0.5 direction= -x
```

Rotate a prism:

```
polyhedron name= prism polygons= {triangle} min= -6 max= 2 \
rotate.angles= {30 60 90}
```

## See Also

[Inserting Polyhedra on page 826](#)

[insert on page 1024](#)

[profile on page 1137](#)

---

## PowerDeviceMode

Sets diffusion models to match the `pd.fermi` model of TSUPREM-4 for power-device applications. It also relaxes time-step controls and reduces mesh refinement around the interfaces.

### Syntax

PowerDeviceMode

### Description

**NOTE** Do not confuse this command with `AdvancedPowerDeviceMode`, which is part of Advanced Calibration. The `PowerDeviceMode` command sets different parameters and meshing criteria similar to TSUPREM-4.

Sentaurus Process and TSUPREM-4 use different code and, sometimes, have different assumptions or algorithms for diffusion. This command tries to minimize these differences by setting appropriate switches that make the results of a Sentaurus Process simulation as close as possible to those produced by TSUPREM-4 with the `pd.fermi` model for boron, phosphorus, arsenic, antimony, and indium in silicon. This includes:

- Switch on Fermi model.
- Switch on solid solubility model.
- Switch on `DopantOnly` charge model.
- Switch on equilibrium activation model for arsenic.
- Switch on segregation model at oxide–silicon interface.
- Switch off dopant and defect clusters.
- Switch off point-defect equations.
- Relax time-step controls by modifying `InitTimeStep`, `deltT`, `delTox`, `delNT`, `IncreaseRatio`, `ReduceRatio`, and `MaxGrowthStep`.
- Switch on TSUPREM-4-style time-step controls.
- Reduce mesh refinement around the interfaces.
- Relax meshing criteria during boundary movement.

---

## print.1d

Prints values along a 1D cross section.

### Syntax

```
print.1d
  [gas]  [interfaces]  [<material>]  [name=<c>]  [region=<c>]
  [syntax.check.value=<c>]
  [x=<n>] [<m>|<cm>|<um>|<nm>]
  [y=<n>] [<m>|<cm>|<um>|<nm>]
  [z=<n>] [<m>|<cm>|<um>|<nm>]
```

### Arguments

gas

By default, gas values are not reported. This argument allows the gas mesh to be included in the extracted data.

interfaces

Prints interface data from the field specified by name. Values from all interfaces are displayed on the screen and are organized by interface. For each point on the interface, a set of numbers is displayed as follows:

- {x value} in one dimension
- {x y value} in two dimensions
- {x y z value} in three dimensions

where x, y, and z are the coordinates of the interface point, and value is the value of the specified field.

<material>

Name of the material for which the data fields are printed.

name

Name of a data field. This allows printing without using the select command. The default is to use the field specified in the most recent select command.

region

Name of the region for which the data fields are printed.

## A: Commands

### print.1d

syntax.check.value

Sets a value to be returned only during syntax-checking mode. Sometimes, the value returned by a command can cause a false syntax-check error because the value returned by the command would not be the value during the normal run mode. Setting this value avoids such problems.

x, y, z

Specify the constant values of a line along which sectioning is performed. In one dimension, these parameters are not necessary. In two dimensions, only one of x or y can be specified for a given device. Specifying x produces a horizontal slice through the device and y specifies a vertical slice. An easy way to remember this is that the cross section is taken at the constant value specified. For a 3D simulation, two of these three arguments must be specified. Default unit:  $\mu\text{m}$ .

## Description

This command is particularly useful for creating input for another xy plot. A Tcl list is returned for all values. This allows subsequent processing (for example, integration) of the resulting profile.

## Examples

Print the selected value at x equal to 1.0  $\mu\text{m}$ :

```
print.1d x= 1.0
```

Print the data field named Arsenic along a vertical line at a lateral position of 1.0  $\mu\text{m}$ :

```
print.1d y= 1.0 name= Arsenic
```

## See Also

[plot.1d on page 1111](#)

[select on page 1168](#)

[tclsel on page 1222](#)

---

## print.data

Writes data in x-, y-, and z-format.

### Syntax

```
print.data
  [name=<c>] [NODE | EDGE] [outfile=<c>]
  [xlo=<n>] [<m>|<cm>|<um>|<nm>] [xhi=<n>] [<m>|<cm>|<um>|<nm>]
  [ylo=<n>] [<m>|<cm>|<um>|<nm>] [yhi=<n>] [<m>|<cm>|<um>|<nm>]
  [zlo=<n>] [<m>|<cm>|<um>|<nm>] [zhi=<n>] [<m>|<cm>|<um>|<nm>]
```

### Arguments

name

Name of a data field. This allows printing without using the `select` command. Default: `Z_Plot_Var`.

NODE, EDGE

Specifies either a node-based field or an edge-based field. Default: NODE.

outfile

Name of output file. The file is opened for writing, and any previous content is destroyed.

xlo, ylo, zlo, xhi, yhi, zhi

Specify a 3D bounding box. Only data within these limits is printed. Default value and unit: 0 μm.

### Description

The file format is the x-position, y-position, and z-position. This command is used primarily to write a data field for use with more sophisticated 3D plotting tools.

### Examples

Print the data field named Boron:

```
print.data outfile= foo name= Boron
```

### See Also

[select on page 1168](#)

**A: Commands**

print\_interpolated\_params

---

## print\_interpolated\_params

Prints the parameters that have already been read and to which mole fraction-dependent interpolation has been applied, and returns them as a Tcl list.

### Syntax

```
print_interpolated_params [Diffuse | KMC | Mechanics]
```

### Arguments

Diffuse, KMC, Mechanics

Prints the mole fraction-dependent parameters containing the chosen option. The option Diffuse prints any unmatched parameters using the other two options. If unspecified, all mole fraction-dependent parameters will be printed.

### Description

This command prints a list of mole fraction-dependent parameters that have been used during the simulation.

The command must be called *after* the expected interpolation has occurred. The interpolated parameter list is created and appended to during the interpolation, for example, during the diffuse command. Therefore, if the print\_interpolated\_params command is called at the beginning of the command file, it will not print anything as the list is empty.

### Examples

Print all mole fraction-dependent parameters used in the simulation:

```
print_interpolated_params
```

Print the mole fraction-dependent parameters containing KMC that were used in the simulation:

```
print_interpolated_params KMC
```

---

## profile

Reads a data file and constructs a data field.

### Syntax

```
profile
  name=<c>
  [Adaptive] [concentration=<n>] [delay.doping.3d] [gaussian.blur]
  [infile=<c>]
  [lateral.function= {xlo= {<n> ...} xhi= {<n> ...} sigma= {<n> ...}}
   LDF.reshaping= {<c> ...}]
  [logarithmic | linear]
  [mask=<n>] [mask.discretization.size=<n>]
  [<material>] [material.specific]
  [max= {<n> <n> <n>}] [min= {<n> <n> <n>}]
  [offset= {<n> <n> <n>}][<m>|<cm>|<um>|<nm>]
  [polyhedron=<c>]
  [region=<c>] [replace | sum]
  [x.sigma=<n>] [xcoord=<n>] [xscale=<n>]
  [y.sigma=<n>] [ymin=<n>] [yscale=<n>] [z.sigma=<n>]
```

### Arguments

#### Adaptive

Specifies whether this profile step is performed with adaptive remeshing. This functionality is not supported when `infile` is a TDR file, or when the `polyhedron` argument is specified. Default: [pdbGet Grid Adaptive].

#### concentration

Specifies the concentration of the field at the specified `xcoord` or inside the specified `polyhedron`. When it is paired with the `xcoord` argument, the `concentration` argument is a list in which the number of list elements must match that of `xcoord`. When it is specified with the `polyhedron` argument, the `concentration` argument is a simple numeric value.

#### delay.doping.3d

Specifies whether the placement of the dopant concentration is delayed until the next remeshing step in the 3D simulation. This may be useful if there are several consecutive `profile` commands, which can be put together and performed in one adaptive remeshing step.

This functionality is not supported when `infile` is a TDR file, or when the `polyhedron` argument is specified. Default: false.

## A: Commands

### profile

#### gaussian.blur

Specifies whether the 2D or 3D doping distribution is generated by combining the 1D depth profile (specified by `infile`) with 2D mask information (specified by `mask`). The lateral distribution is computed by convolving the mask information with the Gaussian function.

#### infile

Name of the file to be read. If it is an ASCII data file, the file must be in a two-column format with depth (in  $\mu\text{m}$ ) in column 1 and the variable in column 2. It also will read the output of the `print .1d` command, which includes Tcl braces for list processing and the material name. If it is a TDR file, it must be in the same dimension as the simulated device structure and requires `.tdr` as the file extension.

#### lateral.function

Specifies the lateral straggling (`sigma`'s) and the lateral distribution function (LDF) for the profile reshaping (`LDF.reshaping`) as a function of depth in a piecewise step manner.

The `xlo`, `xhi`, and `sigma` arguments specify that, between `xlo` and `xhi`, the lateral straggling is `sigma`. These three lists must have exactly the same number of items and must cover the entire depth of the device. For simplicity, however, if `sigma` is a constant (that is, a single value), `xlo` and `xhi` can be omitted.

The `LDF.reshaping` argument specifies the file names of the LDF correction factors in `.plx` file format. The first item of the list specifies the file name for the first pair of `xlo` and `xhi`, and the second item specifies the file name for the second pair of `xlo` and `xhi`, and so on (the file names can be repeated if they are the same). For simplicity, however, if the correction factor is 1 (that is, no correction), the file name can be omitted.

#### logarithmic, linear

Interpolates data using either logarithmic or linear interpolation. The default is `logarithmic`, which is usually more accurate for concentration profiles.

#### mask

Specifies the name of the mask used for Gaussian blurring.

#### mask.discretization.size

During computation of the Gaussian convolution, a 2D mask is divided into small slices in the z-direction. This argument specifies the maximum discretization size for each slice. Default value and unit: 1e-6 cm.

#### <material>

Name of the material to which the field profile is applied. See [Specifying Materials on page 18](#).

`material.specific`

By default, when loading a TDR file, interpolation is material specific, so that data is interpolated from the file only if the material in the existing structure matches. Use `!material.specific` to allow interpolation regardless of material.

`max`

List of numeric values defining the x-, y-, and z- coordinates of the lower-right front corner of the 1D, 2D, or 3D rectangular box into which the profile is imported. For 1D, 2D, and 3D structures, a list of one, two, or three numbers is required, respectively. The possible maximum number is used for missing numbers. Default unit:  $\mu\text{m}$ .

`min`

List of numeric values defining the x-, y-, and z- coordinates of the upper-left back corner of the 1D, 2D, or 3D rectangular box into which the profile is imported. For 1D, 2D, and 3D structures, a list of one, two, or three numbers is required, respectively. The possible minimum number is used for missing numbers. Default unit:  $\mu\text{m}$ .

`name`

Name of the data field. This argument allows for the creation of arbitrary fields, for example, a field called `Measured`.

`offset`

List of numeric values that specify the offsets in the x-, y-, and z-direction, respectively. The missing values are treated as 0. These values will be subtracted from the x-, y-, and z-coordinate, respectively, when creating the data field from the imported field. This argument allows a profile to be shifted. Default value and unit:  $0 \mu\text{m}$ .

`polyhedron`

Specifies a name as defined by the following `polyhedron` command (see [polyhedron on page 1128](#)):

```
polyhedron name=<c> (brick= {...} | original.polyhedron=<c> |
    polygons= {...} | tdr=<c>)
```

If a polyhedron is created by specifying `brick`, you can use different values of standard deviations (`x.sigma`, `y.sigma`, and `z.sigma`) in each of the three principal axes. However, if a polyhedron is created by specified either `tdr` or `polygons`, only a single roll-off function (`x.sigma`) is allowed. The roll-off is computed using the nearest distance to the polyhedron.

`region`

Name of the region to which the profile is applied.

## A: Commands

### profile

replace, sum

These options specify how a newly added profile concentration is used:

- Specify replace to replace the existing dataset with the new concentration of the same name inside the polyhedron or in the rectangular box (specified by the min and max arguments). Outside the polyhedron or the rectangular box, to ensure a smooth transition, the roll-off profile replaces the existing concentration only if the concentration of the roll-off profile is greater than the existing concentration.
- Specify sum to add the new concentration to the matching dataset. This is the default.

x.sigma

Standard deviation of erfc falloff from a rectangular box in the x-direction. It must be specified if a rectangular box or polyhedron is specified. Default unit:  $\mu\text{m}$ .

xcoord

Coordinate in the x-direction where the concentration will be defined. Default unit:  $\mu\text{m}$ .

xscale

The profile command assumes the x-dimension is in micrometers. This argument allows you to scale the depth dimension if necessary. For example, if the depth is in ångströms,  $1\times10^{-4}$  must be specified. Default: 1.0.

y.sigma

Standard deviation of erfc falloff from a rectangular box in the y-direction. If it is not specified, it takes the value of x.sigma. Default unit:  $\mu\text{m}$ .

ymin

Minimum-acceptable value of the data field. Values less than ymin in the data field are set to ymin. This is useful for data that may approach zero when using logarithmic interpolation.

yscale

The scaling factor for the y-dimension (usually, the concentration) of the 1D profile. Default: 1.0.

z.sigma

Standard deviation of erfc falloff from a rectangular box in the z-direction. If it is not specified, it takes the value of y.sigma. Default unit:  $\mu\text{m}$ .

## Description

This command provides different ways of introducing dopant concentration into a device:

- It reads data fields from an ASCII data file or a TDR file, and replaces or adds them to the structure. It allows you to read a doping profile from a SIMS measurement. In this case, if the simulated structure is 2D or 3D, the data field is created uniformly in the lateral direction. This command also allows you to read a field from a TDR file with the same dimension as the simulated structure. You also can limit the extent of the imported profile within a rectangular box by specifying min or max, or both. Outside this box, the profile falls off with a complementary error function (erfc) with standard deviations given by x.sigma, y.sigma, and z.sigma in the x-, y-, and z-direction, respectively.
- It places a uniform dopant concentration inside a polyhedron without triggering remeshing. The dopant and concentration are specified by the name and concentration arguments, respectively. The polyhedron must be already defined using the polyhedron command:

```
polyhedron name=<c> (brick= {...} | original.polyhedron=<c> |
    polygons= {...} | tdr=<c>)
```

If a polyhedron is created by specifying brick, you can use different values of standard deviations (x.sigma, y.sigma, and z.sigma) in each of the three principal axes. However, if a polyhedron is created by specifying either tdr or polygons, only a single roll-off function (x.sigma) is allowed. The roll-off is computed using the nearest distance to the polyhedron.

- It computes a 2D or 3D dopant distribution by combining a 1D depth profile (specified by either infile or both the xcoord and concentration arguments) and 2D mask information. The 1D depth profile is obtained elsewhere (for example, a 1D process simulation or from a SIMS profile) and is stored in a file specified by infile in ASCII format. The 2D lateral dopant profile is generated by convolving the mask with a Gaussian function in two dimensions<sup>1</sup>, essentially smoothing the sharp edges of the mask. Depth-dependent lateral straggling and profile reshaping are specified as lists inside the lateral.function argument. The doping profile placement can be adaptive or nonadaptive. In three dimensions and with Adaptive specified, you can delay the profile placement until the next remeshing step by specifying the delay.doping.3d option.

## Examples

Read a boron profile from a Monte Carlo ion implantation. Scale the depth by  $1\times10^{-4}$  to convert ångström to micrometer:

```
profile name= Boron infile= utmar.bor xscale= 1.0e-4
```

---

1. For more information, go to [https://en.wikipedia.org/wiki/Gaussian\\_blur](https://en.wikipedia.org/wiki/Gaussian_blur).

## A: Commands

### profile

Read a file named `SIMS` into a data field called `Data`. This can be performed to initialize a device doping profile or to read in a measured profile that is the target of a diffusion extraction:

```
profile name= Data infile= SIMS
```

Assign a phosphorus concentration of  $1\text{e}21 \text{ cm}^{-3}$  to nodes inside the brick as specified by the minimum and maximum coordinates  $\{0.0 \text{ } -0.5 \text{ } -0.5 \text{ } 0.5 \text{ } 0.5 \text{ } 0.5\}$  with different roll-offs in the three principal axes:

```
polyhedron name= mypoly brick= \{0.0 -0.5 -0.5 0.5 0.5 0.5\}
profile name= Phosphorus polyhedron= mypoly concentration= 1e21 x.sigma= 0.1 \
y.sigma=0.2 z.sigma=0.3
```

Assign a boron concentration of  $1\text{e}20 \text{ cm}^{-3}$  to nodes inside the polyhedron as specified by the `mypolyhedron.tdr` file with a single erfc roll-off function:

```
polyhedron name= mypoly tdr= mypolyhedron.tdr
profile name= Boron polyhedron= mypoly concentration= 1e20 x.sigma= 0.1
```

Compute the boron distribution by multiplying the 1D depth profile (`1dplx`) with the 2D mask and Gaussian convolution. Specify the lateral `sigma=0.12` everywhere above  $0.1 \mu\text{m}$  and `sigma=0.15` below  $0.1 \mu\text{m}$  down to the bottom of the structure ( $x = 50 \mu\text{m}$ ). Apply profile reshaping to the first sigma, and delay the doping profile placement until the next remeshing step:

```
profile name=Boron infile=1dplx mask=complex gaussian.blur \
Adaptive delay.doping.3d \
lateral.function= \{xlo= \{-1.0 0.1\} xhi= \{0.1 50.0\} sigma= \{0.12 0.15\}\} \
LDF.reshaping= \{ldfplx\}
```

### See Also

[print.1d on page 1133](#)

---

## RangeRefineboxes

Creates a set of refinement boxes based on a mask, and a set of range and extent parameters. All boxes share a set of global refinement settings, but each box can have additional local refinement settings.

### Syntax

```
RangeRefineboxes
  boxes= {
    drange=<drange1> [<box-specific_arguments>]
    [drange=<drange2> [<box-specific_arguments>]]
    ...
  }
  mask=<c>
  name=<c>
  range=<c>
  [<other_arguments>]
```

### Arguments

<box-specific\_arguments>

Any argument of the `refinebox` command. These arguments are applied only to the individual refinement box. They can overwrite global parameters defined in the `<other_arguments>` section.

boxes

A Tcl list containing a set of Tcl lists. Each Tcl list contains specific parameter settings for one individual refinement box.

drange

Specifies the primary extent of an individual refinement box, which extends from `xmin = range - drange` to `xmax = range + drange`.

mask

Specifies the mask under which the refinement is to be applied.

name

Specifies the root name for the set of refinement boxes. Each individual refinement box inherits a name of the form `<c>_<n>`, where `<c>` is the value of the `name` argument and `<n>` is a counter.

## A: Commands

### RangeRefineboxes

<other\_arguments>

Any valid argument of the `refinebox` command.

`range`

Specifies the center of the primary extent for all refinement boxes in the set. For example, you can use `range` from an implant table to define a set of refinement boxes to resolve the area that dopants penetrate in a subsequent implantation step.

## Description

The refinement is applied to the area under the specified mask. The lateral extent is controlled by the same arguments as in the `refinebox` command, for example, `mask.edge.refine.extent` and `mask.edge.mns`.

The primary extent is defined by `range` and `drange`. The `range` argument is common to all refinement boxes and may be taken as the `range` argument for a given implantation. The `drange` argument can be set for each related refinement box separately.

As optional global default arguments, any argument from the `refinebox` command is allowed. These arguments are applied to all refinement boxes of the set. For each individual refinement box, an additional `refinebox` command can be set, which can overwrite globally defined arguments or add new arguments. There are no limits on how many refinement boxes can be in the set. The individual refinement boxes inherit the root name (specified by the `name` argument) with a numeric suffix counter.

**NOTE** The `RangeRefineboxes` command makes one call to the `refinebox` command per individual refinement box.

**NOTE** You can use the `DeleteRefinementboxes` command to remove the entire set of refinement boxes created with the `RangeRefineboxes` command.

## Examples

Create a set of refinement boxes:

```
mask name= M1_p segments= {6 10}
array set moments [implant Arsenic dose= 5e13<cm-2> energy= 1000<keV> \
    tilt= 0 rotation= 0 get.moments]
set range $moments(rp)
set sigma $moments(stdev)
eval RangeRefineboxes name= "RM1" mask= "M1_p" range= $range \
    boxes= \\{ \
        {drange= $sigma xrefine= [expr $sigma/4.0] yrefine= [expr $sigma/4.0] \
            extend= 0} \}
```

```
{drange= [expr 4*$sigma] xrefine= $sigma yrefine= $sigma \
    extend= [expr 2*$sigma]} \
{drange= [expr 2*$sigma] mask.edge.mns= [expr $sigma/8.0] \
    mask.edge.refine.extent= [expr 2*$sigma] mask.edge.ngr= 1} } \
extend= 1.0 xrefine= 0.5 yrefine= 0.5 info= 2
```

## See Also

[DeleteRefinementboxes on page 927](#)  
[refinebox on page 1151](#)

## A: Commands

reaction

---

# reaction

Defines reacting materials and the new material that forms as the product of the reaction.

## Syntax

```
reaction
(
    list |
    (lkmc [ambient.products= <list>] [ambients= <list>] [energy=<n>]
     [extra.sites=<n>] [mat.lattice.lkmc=<c>] [max.site.separation=<n>]
     [nucleation.material=<c>] [prefactor=<n>] [print]
     [products= <list>] [products.efactor=<n>]
     [reactants= <list>] [reactants.efactor=<n>] [segregation= <list>]) |
    mat.l=<c> mat.r=<c> mat.new=<c> name=<c>
)
[alt.matername=<c>] [ambient.name=<c>] [clear] [delete]
[diffusing.species= <list>]
[mat.final=<c> new.like=<c>] [multiphase]
```

## Arguments

alt.matername

Specifies an alternative material to mat .new if a native layer is deposited in a reaction. This argument takes effect only with the setting:

```
pdbSet Grid Alternative.NativeLayer 1
```

ambient.name

Specifies an ambient-type reaction and which ambient must be present for this reaction to occur.

ambient.products

Specifies the ambient that will be the by-product of the reaction. This affects the incoming ambient flux in the Coordinations.Reactions model. For example:

```
ambient.products= {HGas=1}
```

ambients

Specifies a list of ambients along with the stoichiometry for LKMC reactions in the Coordinations.Reactions model. For example:

```
ambients= {SiHStar=1}
```

clear

If a reaction is named, this argument clears the diffusing species list from that reaction. If no reaction is named, it deletes all reactions (may only be useful in special situations).

delete

Deletes the named reaction.

diffusing.species

List of reactants for material growth reactions either ambient type or nonambient type. For ambient-type reactions, the (one only) default diffusing species name is the ambient name, but it can be changed using this argument. For nonambient reactions (such as silicidation), multiple diffusing species can be listed. Reactants are added automatically to the global solution list in the `SetReactantSolutions` procedure.

energy

Sets an additional energy barrier for LKMC reactions when using the `Coordinations.Reactions` model (see [Reaction Rates in the Coordinations.Reactions Model on page 578](#)).

extra.sites

Usually, LKMC reactions are created if there are sufficient valid sites for the reaction products within the `max.site.separation` distance. The `extra.sites` argument can be used to obtain additional valid sites to account for intermediate reactions without the need to create additional reactions.

list

Lists the names of the already defined reactions.

mat.final

For reactions that use a temporary material during growth, `mat.final` can be set to convert the temporary material to a final material after the diffuse step is finished. This is usually used with epitaxial reactions to keep regions separated during growth and only merged afterwards.

mat.l, mat.r

Specify the material names for each side (left and right) of the interface before the reaction.

mat.lattice.lkmc

Material used for lattice creation in LKMC.

## A: Commands

### reaction

mat.new

Specifies a valid material name as the product of the reaction.

max.site.separation

Specifies the maximum reaction distance. Reactants on the surface must be separated by less than this distance for a reaction to occur. In addition, reaction products must have valid sites separated by less than this distance. The default is 0.41 nm, which is between the next nearest neighbor and the third nearest neighbor distances.

multiphase

Specify this option to switch on a multiphase reaction such as silicidation of nickel.

name

Name of the reaction. The argument name is used to identify the reactions during the growth process.

new.like

Name of the existing material that the new material is behaving like. This includes the existing material and other material interfaces. It is performed in the ReactantLike procedure.

nucleation.material

Material on which nucleation occurs during nonselective epitaxy in LKMC.

prefactor

Sets the LKMC reaction prefactor when using the Coordinations.Reactions model (see [Reaction Rates in the Coordinations.Reactions Model on page 578](#)). Default: 1.01.

print

Prints a list of reactions with their settings. If lkmc is specified, this argument only prints LKMC reactions with settings.

products

Specifies a list of products along with the stoichiometry for LKMC reactions in the Coordinations.Reactions model. For example:

```
products= {Silicon=1 HStar=1}
```

products.efactor

Sets a multiplicative factor for the contribution of the formation energy of the products to the reaction energy (see [Reaction Rates in the Coordinations.Reactions Model on page 578](#)). Default: 1.0.

reactants

Specifies a list of reactants along with the stoichiometry for LKMC reactions in the Coordinations.Reactions model. For example:

```
reactants= {Silicon=1 HStar=2}
```

reactants.efactor

Sets a multiplicative factor for the contribution of the formation energy of the reactants to the reaction energy (see [Reaction Rates in the Coordinations.Reactions Model on page 578](#)). Default: -1.0.

segregation

Specifies a pair of reactants that participate in a two-site exchange segregation reaction. For example:

```
segregation= {Silicon Germanium}
```

## Description

This command is used to specify either reactions for continuum moving-boundary simulations (such as oxidation, silicidation, and epitaxy) or LKMC chemical vapor epitaxy reactions (such as adsorption, surface reaction, desorption, and etching). For more information about LKMC reactions, see [Coordinations.Reactions Model on page 576](#).

The convention for interface materials is `mat1_mat2` where the materials are ordered alphabetically. For the purpose of this command, left refers to `mat1` and right refers to `mat2`. Both materials must be specified when using this command. Silicidation and oxidation rely on this information.

## Examples

Define a reaction named `MyDryOx`. The reaction will occur at the gas–silicon interface and the new material will be oxide. For the reaction to occur, O2 must be present in the structure. It is expected that you will provide the actual reaction equation for the interface using the Alagator language:

```
reaction name= MyDryOx mat.l= Silicon mat.r= Gas mat.new= oxide \
diffusing.species= O2
```

## A: Commands

### reaction

In this example, silicon and titanium are the reacting materials. The product of the reaction is titanium silicide. Two species, silicon and titanium, are needed for the reaction. It is expected that you will provide the actual reaction equations for the interface using the Alagator language:

```
reaction name= silicidation mat.l= Silicon mat.r= Titanium \
mat.new= TiSilicide diffusing.species= {Silicon Titanium} new.like= oxide
```

### See Also

[Basics of Specifying Generic Growth Equations on page 612](#)

---

## refinebox

Sets the local grid parameters and performs a grid refinement using the MGOALS module.

### Syntax

```
refinebox
  [3d]  [Adaptive]  [clear]  [double.side]
  [kmc]  [list]
  [(mask=<c> extrusion.min=<n> extrusion.max=<n>)  [extend=<n>]
   ([mask.corner.mns=<n>]  [mask.corner.ngr=<n>]
    [mask.corner.refine.extent=<n>]  |
     [mask.edge.mns=<n>]  [mask.edge.ngr=<n>]  [mask.edge.refine.extent=<n>]))
  [<material>]  [materials= <list>]
  [max= <list>]  [min= <list>]
  [name=<c>]
  [print]
  [regions= <list>]
  [xrefine= <list>] [<m>|<cm>|<um>|<nm>]
  [yrefine= <list>] [<m>|<cm>|<um>|<nm>]
  [zrefine= <list>] [<m>|<cm>|<um>|<nm>]

  [interface.mat.pairs= <list>]
  [interface.materials= <list>]
  [interface.region.pairs= <list>]
  [interface.regions= <list>]
  [max.lateral.size=<n>] [<m>|<cm>|<um>|<nm>]
  [min.normal.size=<n>] [<m>|<cm>|<um>|<nm>]
  [normal.growth.ratio=<n>]
  [offsetting]
  [offsetting.maxlevel=<i>]

  [DelPSC
    [interface.mat.pairs= <list>]
    [interface.materials= <list>]
    [interface.region.pairs= <list>]
    [interface.regions= <list>]
  ]
  [abs.error= {<field1>=<n> <field2>=<n> ...}]
  [def.abs.error=<n>]
  [def.max.asinhdiff=<n>]
  [def.max.difference=<n>]
  [def.max.dose.error=<n>]
  [def.max.gradient=<n>]
  [def.max.logdiff=<n>]
  [def.rel.error=<n>]
```

## A: Commands

refinebox

```
[max.asinhdiff= {<field1>=<n> <field2>=<n> ...}]\n[max.difference= {<field1>=<n> <field2>=<n> ...}]\n[max.dose.error= {<field1>=<n> <field2>=<n> ...}]\n[max.gradient= {<field1>=<n> <field2>=<n> ...}]\n[max.logdiff= {<field1>=<n> <field2>=<n> ...}]\n[max.value=<n>] [min.value=<n>]\n[refine.add.fields= <list>]\n[refine.dir.factor= <list>]\n[refine.expr=<c>]\n[refine.field.expr= {<field1>=<c> <field2>=<c> ...}]\n[refine.fields= <list>]\n[refine.max.edge= <list>]\n[refine.min.edge= <list>]\n[refine.rm.fields= <list>]\n[refine.type=<c>]\n[rel.error= {<field1>=<n> <field2>=<n> ...}]\n[target.length=<n>] [<um>] [target.length.scaling=<n>]
```

## Arguments

3d

Specifies the refinement box for only three dimensions, or for only one dimension and two dimensions. The default behavior is to always apply the refinement box. If 3d is specified, the refinement box only applies to three dimensions. If !3d is specified, the refinement box only applies to one dimension and two dimensions.

Adaptive

Specifies an adaptive refinement box. Adaptive refinement boxes are used during all remeshing operations (such as deposit, etch, photo, transform) but will not be used during solve unless adaptive meshing is switched on (by using pdbSet Grid Adaptive 1).

clear

When used without other arguments, clear deletes all previously defined refinement boxes. When used with name, only the named refinement box is deleted.

double.side

If !double.side is specified with offsetting, Sentaurus Mesh interprets interface.mat.pairs and interface.region.pairs in a nonsymmetric fashion. The default is double.side, that is, the specification of a material or region pair  $x_1/x_2$  is interpreted by Sentaurus Mesh as if the parameters were defined symmetrically for both  $x_1/x_2$  and  $x_2/x_1$ .

extend

Optional extension when using a mask-driven refinement. This value can be positive (or negative) and extends (shrinks) the refinement isotropically in y and z. The original mask remains unchanged. Default unit:  $\mu\text{m}$ .

extrusion.max, extrusion.min

Maximum and minimum coordinates in the x-axis where the refinement will be applied when using `mask`. Default unit:  $\mu\text{m}$ .

kmc

Refines the internal KMC boxes only.

list

Lists the defined refinement boxes.

mask

Uses an existing mask name as an extra constraint to where the refinement will be applied. If the refinement contains another spatial constraint (for example, using `min` and `max`), the final application region is the intersection of the other constraints and the specified extruded mask.

This argument requires specifying the box length in x (lacked by the mask) using `extrusion.min` and `extrusion.max`, and optionally allows the use of `extend`, which allows for the definition of layout (mask)-driven refinements.

mask.corner.mns

Specifies the minimum mesh size near the mask corner (actual edge length may be up to two times smaller than this setting). This argument must be used with `mask.corner.refine.extent` to have an effect. Default unit:  $\mu\text{m}$ .

mask.corner.ngr

Specifies the growth rate of refinement away from the mask corner. This argument must be used with `mask.corner.refine.extent` to have an effect. Default value and unit:  $1.0 \mu\text{m}$  (no growth).

mask.corner.refine.extent

Specifies the distance from the mask corner over which corner-based refinement occurs. It must be specified to obtain mask corner-based refinement. Default unit:  $\mu\text{m}$ .

## A: Commands

refinebox

mask.edge.mns

Specifies the minimum mesh size near the mask edge (actual edge length may be up to two times smaller than this setting). This argument must be used with mask.edge.refine.extent to have an effect. Default unit:  $\mu\text{m}$ .

mask.edge.ngr

Specifies the growth rate of refinement away from the mask edge. This argument must be used with mask.edge.refine.extent to have an effect. Default value and unit: 1.0  $\mu\text{m}$  (no growth).

mask.edge.refine.extent

Specifies the distance from the mask edge over which edge-based refinement occurs. It must be specified to obtain mask edge-based refinement. Default unit:  $\mu\text{m}$ .

<material>

Limits the refinement box to a particular material. By default, the refinement box applies to all materials. See [Specifying Materials on page 18](#).

materials

Limits the refinement box to a list of materials. By default, the refinement box applies to all materials. See [Specifying Materials on page 18](#).

max, min

Limits the extent of the refinement box. Both arguments take a Tcl list of numbers defining the refinement box extent in the x-, y-, and z-axes. You can specify either one or both min and max with a Tcl list of one, two, or three numbers for each argument. If one number is specified, it is taken to be the limit in the x-axis. If two numbers are specified, they set limits for the x-axis and y-axis. Similarly, three numbers specify a limit in all three axes. Default unit:  $\mu\text{m}$ .

name

Name of the refinement box.

print

Prints information for all refinement boxes. If name is specified, only the named refinement box information is printed.

regions

Limits the refinement box to a list of regions. By default, the refinement box applies to all regions.

xrefine

List of three numbers defining the element sizes in the x-direction at the top, middle, and bottom of the box. Default unit:  $\mu\text{m}$ .

yrefine

List of three numbers defining the element sizes in the y-direction at the left, middle, and right of the box. Default unit:  $\mu\text{m}$ .

zrefine

List of three numbers defining the element sizes in the z-direction at the front, middle, and back of the box. Default unit:  $\mu\text{m}$ .

### **Arguments: Interface Refinement Control**

interface.mat.pairs

A set of pairs of materials where interface meshing will be switched on (1st and 2nd, 3rd and 4th, and so on).

interface.materials

All interfaces that contain any of the materials listed here are refined using the min.normal.size criterion. By default, in two dimensions, interface refinement is applied to all interfaces of Silicon, Polysilicon, or Oxide. In three dimensions, interface refinement is only by default applied to interfaces of Silicon.

interface.region.pairs

A set of pairs of regions where interface meshing will be switched on (1st and 2nd, 3rd and 4th, and so on). This region-based interface specification is supported only for Sentaurus Mesh offsetting, that is, when offsetting also is given.

interface.regions

Used only in conjunction with offsetting or offsetting.maxlevel to switch on Sentaurus Mesh offsetting or to specify offsetting.maxlevel on a regionwise basis for Sentaurus Mesh offsetting.

max.lateral.size

Specifies the maximum lateral spacing at the interface. Default unit:  $\mu\text{m}$ .

min.normal.size

Specifies the minimum edge spacing at interfaces for this box. Default unit:  $\mu\text{m}$ .

## A: Commands

refinebox

normal.growth.ratio

Specifies the edge-to-edge growth ratio moving away from an interface.

offsetting

When offsetting is specified along with interface.materials, interface.mat.pairs, interface.regions, or interface.region.pairs, the Sentaurus Mesh offsetting algorithm is used to generate offsetting layers at the given interface.

offsetting.maxlevel

Specifies the number of offsetting layers at the interface when Sentaurus Mesh offsetting is used, specified either by material or region using interface.materials or interface.regions, respectively.

## Arguments: Boundary Rediscretization Using DelPSC Algorithm

DelPSC

Specify this option to apply the Delaunay refinement for piecewise smooth complex (DelPSC) algorithm to rediscretize curved surfaces on the boundary at the beginning of the Sentaurus Mesh simulation. This is equivalent to the following setting:

```
pdbSet Grid SnMesh Apply.Brep.DelPSC true
```

interface.mat.pairs

Restricts the application of the DelPSC algorithm to interfaces specified by pairs of materials (first and second, third and fourth, and so on). For example:

```
interface.mat.pairs= {Silicon Oxide}
```

interface.materials

Restricts the application of the DelPSC algorithm to interfaces of the specified materials. For example:

```
interface.materials = {Silicon}
```

interface.region.pairs

Restricts the application of the DelPSC algorithm to interfaces specified by pairs of regions (first and second, third and fourth, and so on). For example:

```
interface.region.pairs= {Substrate field_ox}
```

interface.regions

Restricts the application of the DelPSC algorithm to interfaces of the specified regions. For example:

```
interface.regions= {Substrate}
```

### **Arguments: Adaptive Meshing**

abs.error

Sets a field-dependent value of the minimum significant field value.

def.abs.error

Sets the field-independent default value of the minimum significant field value.

def.max.asinhdiff

Sets the field-independent default value of the maximum inverse hyperbolic sine (asinh) difference criteria.

def.max.difference

Sets the field-independent default value of the maximum absolute difference criteria.

def.max.dose.error

Sets the field-independent default value of the maximum local dose error criteria.

def.max.gradient

Sets the field-independent default value of the maximum gradient criteria.

def.max.logdiff

Sets the field-independent default value of the maximum logarithmic difference criteria.

def.rel.error

Sets the field-independent default value of the required relative change of a field across an edge.

max.asinhdiff

Sets a field-dependent value of the inverse hyperbolic sine difference criteria.

max.difference

Sets a field-dependent value of the maximum absolute difference criteria.

## A: Commands

refinebox

max.dose.error

Sets a field-dependent value of the maximum local dose error criteria.

max.gradient

Sets a field-dependent value of the maximum gradient criteria.

max.logdiff

Sets a field-dependent value of the maximum logarithmic difference criteria.

max.value

Maximum interval value for interval refinement.

min.value

Minimum interval value for interval refinement.

refine.add.fields

List of fields to be added to the default list of fields considered for adaptive refinement.

refine.dir.factor

Applies adaptive refinement more strongly in one direction than another. A factor of 1 has no effect. A factor less than 1 causes smaller edges in that direction.

For example, `refine.dir.factor= { 0.1 1.0 }` requests that, for a given adaptive refinement expression value, edges in the x-direction be 10 times smaller than edges in the y-direction.

refine.expr

Specifies a refinement expression. It takes any valid Alagator expression that produces a node-based result.

**NOTE** Earlier releases required the `diff()` operator, but now, the `diff` operator must not be used. Similar results can be obtained for earlier releases by removing the `diff` operator.

refine.field.expr

Sets a field-dependent refinement expression.

refine.fields

Replaces the default list of fields considered for adaptive refinement. Solution variables and terms can appear in the `refine.fields` list. (For a description of a term, see [term on page 1232](#).) The default list includes all dopants and point defects.

`refine.max.edge`

Sets the direction-dependent maximum edge length.

`refine.min.edge`

Sets the direction-dependent minimum edge length.

`refine.rm.fields`

Removes the specified fields from the default list of fields considered for adaptive meshing.

`refine.type`

Specifies the type of criteria to apply for adaptive refinement. Allowed values are `interval` and `error` (default).

`rel.error`

Sets a field-dependent value of the required relative change of the refined field across an edge.

`target.length`

Target length for interval refinement. Default unit:  $\mu\text{m}$ .

`target.length.scaling`

Scaling factor used in the calculation of the effective target length for interval refinement.

## Description

This command specifies mesh refinement. The following types of refinement box are available:

- Standard: Independent `xrefine`, `yrefine`, `zrefine` settings.
- Interface: Refinement near one or more interfaces.
- Adaptive: Adaptive refinement on fields.
- Plane: Planar refinement for crystal boundaries.
- Bulk mask: Confine refinement to an extruded boundary defined by a mask.
- Mask edge: Confine refinement to a specified distance from a specified mask.

All refinement boxes can be limited by material or spatially by specifying x-, y-, or z- minimum or maximum limits.

## A: Commands

refinebox

### Examples

Define two refinement boxes:

```
refinebox min= {-0.25 0.4} max= {0.4 0.6} xrefine= {0.1 0.06 0.1} \
    yrefine= {0.1 0.01 0.1} oxide
refinebox min= {0.6 0.6} max= {0.8 0.8} xrefine= {0.1 0.03 0.1} \
    yrefine= {0.1 0.03 0.1} silicon
```

Create an adaptive refinement box that applies maximum dose error criteria to the default list of adaptive species, and effectively switch off relative error criteria, which is on by default:

```
refinebox adaptive def.rel.error= 100 def.max.dose.error= 5e9
```

Form the boundary for the refinement by extending (by 0.2 μm) an existing mask called Mask1 extruded from 0 μm to 0.05 μm:

```
polygon name= pol segments= {- .5 -.5 .5 -.5 .5 .5 0 .5 0 0 -.5 0}
mask name= Mask1 polygons= {pol}
refinebox name= "ref1" mask= Mask1 yrefine= {0.05 0.075 0.075} \
    extrusion.min= 0 extrusion.max= 0.05 extend= 0.2
```

### See Also

[Mesh Refinement on page 722](#)

[mask on page 1065](#)

[mgoals on page 1083](#)

---

## region

Creates regions, marks substrates, and changes region materials.

### Syntax

```
region
  <material>
    xlo=<c> [ylo=<c>] [zlo=<c>]
    xhi=<c> [yhi=<c>] [zhi=<c>]
    [alt.matername=<c>] [bbox | bbox.cm | bbox.um]
    [change.material] [cropped.bbox] [exact.name]
    [field=<c> (resistivity=<n>[<ohm-cm>] | concentration=<n>)]
    [left | right | back | front | top | bottom]
    [list | list.bulk | list.gas | list.interface]
    [material]
    [max= {<n> <n> <n>} min= {<n> <n> <n>}]
    [name=<c>] [new.name=<c> point= {<n> <n> <n>}]
    [substrate] [syntax.check.value=<c>] [volume] [zero.data]
```

### Arguments

alt.matername

Specifies the name of the material that should be written in the TDR file for regions of the newly defined material.

For example, when writing the TDR file, if the newly defined material is called MySilicon and alt.matername=Silicon, Sentaurus Process uses Silicon for those regions of MySilicon.

This is useful when transferring the structure to device simulation.

bbox, bbox.cm, bbox.um

If specified, the region command returns the maximum extents of the region in two points. If bbox.cm is specified, it returns the maximum extents of the region in centimeter. If bbox.um is specified, it returns the maximum extents of the region in micrometer.

change.material

Changes the material of an existing region (must be used with name). Changing the material of selected regions (to and from gas) can be used to change the structure without remeshing. Meshes of material gas are ignored in most process steps: implantation and oxidation.

## A: Commands

region

concentration

Specifies the value of the field directly. Default unit: cm<sup>-3</sup>.

cropped.bbox

If specified, returns the cropped bounding box of a region that lies within a user-specified bounding box.

exact.name

Usually when changing the material of a region, all ancestors of the named region (if there are any) are converted as well as the named region if it exists (see [Regionwise Parameters and Region Name-Handling on page 29](#)).

If exact.name is switched on, only a region whose name exactly matches the name argument will have its material changed. Default: false.

field

Name of a field to be initialized within this region.

left | right | back | front | top | bottom

If specified, returns the region names on either the left, right, back, front, top, or bottom of the structure.

list, list.bulk, list.gas, list.interface

Used to obtain a Tcl list of regions:

- list returns a list of all regions.
- list.bulk returns a list of nongas, noninterface regions (that is, all bulk regions).
- list.gas returns a list of gas regions.
- list.interface returns a list of interface regions.

<material>

Material of the region. See [Specifying Materials on page 18](#).

material

If specified, it returns the material name of the named region.

max, min

User-specified bounding box.

name

Name of the region. The name must not contain an underscore (\_) or a period (.) because these characters have special meaning. The name must be different than an existing material name (see [Regionwise Parameters and Region Name-Handling on page 29](#)).

new.name, point

Used together to change the name of a region, where point must specify a point (a list of doubles) within a region. The point must not be on or very near a border. The argument new.name specifies the new name of the region. The name must be different than an existing material name (see [Regionwise Parameters and Region Name-Handling on page 29](#)).

resistivity

Sets the value of the field by requesting a resistivity. This argument only works for fields that have the resistivity parameters in the PDB (which by default is only As, B, P, Sb, and In in silicon).

substrate

Tags a named region as the substrate for subsequent analysis. Setting !substrate clears the substrate tag. If no region name is specified and !substrate is set, all substrate tags are cleared.

syntax.check.value

Sets a value to be returned only during syntax-checking mode. Sometimes, the value returned by a command can cause a false syntax-check error because the value returned by the command would not be the value during the normal run mode. Setting this value avoids such problems.

xlo, ylo, zlo, xhi, yhi, zhi

Specify the bounds of the region. The <c> value must be one of the tags created in a preceding line command.

volume

If specified, the region command returns the volume of the named region. The units will be in cm<sup>D</sup>, where D is the simulation dimension.

zero.data

Usually when the material of a region is changed using change.material, all data in that region is set to 0. Setting !zero.data leaves the data untouched. The default value for this parameter is taken from pdbGet Grid default.zero.data, which allows a global setting for this argument.

## A: Commands

### region

#### Description

The `region` command has different applications:

- At the beginning of a simulation, the initial regions are created with the `region` command in concert with the `line` command and the `init` command. The `line` command defines where mesh lines go.
- The `region` command specifies between which mesh lines the regions are created and what material the regions will be, and whether this region will be a substrate. It is used to change the material of a region at any point in the simulation after the structure has been initialized.
- The `region` command can be used to return a cropped bounding box of a region, specified within a user-specified bounding box, defined by `min` and `max` along with a region name.

#### Examples

Create a new material `MySilicon`, and then change the material of a region named `bulk` to `MySilicon` without changing the data:

```
mater name= MySilicon new.like= Silicon add  
region name= bulk MySilicon change.material !zero.data
```

Change the region `Gate` to `Gas` before setting all fields to zero in `Gate` (`zero.data` defaults to true):

```
region name= Gate Gas change.material
```

Create a 2D silicon region using the statements from the example for the `line` command:

```
region silicon ylo= left yhi= right xlo= surf xhi= back
```

Return a cropped bounding box of the region `bulk` that lies within the specified bounding box defined by `min` and `max`:

```
region name= bulk min= {-5.0 0.0 0.0} max= {5.0 1.0 1.0} cropped.bbox
```

#### See Also

[integrate on page 1027](#)

[line on page 1053](#)

---

## sde

Dispatches commands to Sentaurus Structure Editor (only available for 3D simulations).

### Syntax

```
sde
{<Sentaurus Structure Editor commands>}
[Adaptive] [external] [logfile=<c>] [off] [on]
[polyhedron=<c>] [polyhedron.material=<c>]
[remesh] [SdeCheck]
```

### Arguments

#### Adaptive

If specified, Adaptive switches on adaptive meshing if remesh is given. Parameters for adaptive meshing are described in [Adaptive Mesh Refinement on page 729](#). The default is the return value of pdbGet Grid Adaptive.

#### external

Puts the Sentaurus Structure Editor interface in external mode, which can be used to create polyhedra to be inserted into a Sentaurus Process structure using the 3D MGOALS mode. When the external mode is switched on, all geometry transformations such as etching and deposition are applied to the external Sentaurus Structure Editor structure (see [Insertion: External Mode on page 827](#)).

#### logfile

Name of the file that will log all the Scheme commands dispatched to Sentaurus Structure Editor. The recommended file extension is .scm. The file will contain both the Scheme commands translated from Sentaurus Process etch, deposit, strip, photo, and transform commands, and the user-specified Scheme commands inside the sde command.

The log file can be used for fine-tuning and debugging in a standalone run of Sentaurus Structure Editor such as:

```
sde -l mylogfile.scm
```

#### off

Switches off the Sentaurus Structure Editor mode if it has been switched on previously. By default, the Sentaurus Structure Editor mode is off. Operations will be performed by MGOALS instead.

## A: Commands

sde

on

Switches on Sentaurus Structure Editor for 3D geometry modeling.

polyhedron

Used for external mode only (see `external`). This polyhedron is used to initialize the external Sentaurus Structure Editor interface. The material to be used for this polygon is chosen using `polyhedron.material`.

`polyhedron.material`

Selects the material of the polyhedron that is used to initialize the external mode (see `external` and `polyhedron`). Default: Silicon.

remesh

Forces a remesh at the end of the `sde` command.

<Sentaurus Structure Editor commands>

Any number of `sde` commands in the Scheme scripting language. You must enclose the Scheme commands in a pair of braces to protect them from the Tcl command interpreter. The opening brace must be on the same line as the `sde` command, for example:

```
sde {  
    (sdepe:depo "thickness" 0.01 "type" "iso" "algorithm" "pt"  
        "max-chamfer-angle" 30 "steps" 1 "material" "Oxide")  
    (sdeio:save-tdr-bnd "all" "out1_sde.tdr")  
}
```

**NOTE** Commands to orientate Sentaurus Structure Editor based on Sentaurus Process settings are sent first through the interface before user commands. These settings can be deleted if `sde:clear` is specified. Therefore, never specify `sde:clear` in this set of commands.

SdeCheck

Performs a geometry check of every boundary file that is created by Sentaurus Structure Editor. This helps to detect failures in the geometry-modeling part and prevents the Sentaurus Process simulation from continuing after an incorrect boundary representation is found.

## Description

This command enables and configures the interface between Sentaurus Process and Sentaurus Structure Editor. When `sde on` is specified, all 3D geometry modeling is performed using Sentaurus Structure Editor. Sentaurus Process will translate geometry-modifying commands to

the Sentaurus Structure Editor language and retrieve the resulting modified structure when necessary. The supported commands are `deposit`, `etch`, `photo`, `strip`, and `transform`.

**NOTE** Scheme commands can be sent directly to Sentaurus Structure Editor using the `sde` command, but they must be enclosed in a pair of braces to prevent syntax errors in the Tcl interpreter. Several Scheme commands can be specified inside one `sde` command; each of them must start on a new line.

## Examples

Enable the use of Sentaurus Structure Editor or geometry modeling, specify the log file for the Scheme commands, and check all boundary files written by Sentaurus Structure Editor:

```
sde logfile= depo.scm on SdeCheck  
pdbSet InfoDefault 1
```

Create a cuboid in Sentaurus Structure Editor with tapered sidewalls and save the structure to a TDR file:

```
sde {  
    (sdegeo:set-default-boolean "ABA")  
    (define r1 (sdegeo:create-cuboid (position 0 0.6 0)  
                                       (position 0.2 0.3 0.5) "Silicon" "Silicon_2"))  
    (define facelist (list (car (find-face-id (position 0.1 0.3 0.25)))  
                           (car (find-face-id (position 0.2 0.5 0.25)))))  
    (sdegeo:taper-faces facelist (position 0.2 0.3 0.5) (gvector 0 0 1) 5)  
    (sdeio:save-tdr-bnd "all" "out1_sde.tdr")  
}
```

## See Also

For details about Scheme commands, refer to the *Sentaurus™ Structure Editor User Guide*.

## A: Commands

select

---

# select

Selects the variable for display in all postprocessing commands.

## Syntax

```
select
  [delete] [edge.vector] [element] [interfaces]
  [list] [list.all] [<material>]
  ([min | max] | [report.location])
  [name=<c>] [node.evaluate] [permanent] [present]
  [region=<c>] [store] [syntax.check.value=<c>] [value=<c>] [z=<c>]
```

## Arguments

delete

Deletes the data field specified by name.

edge.vector

Computes the weighted field with respect to the edge orientation strongly favoring axis-oriented edges. Used with adaptive meshing.

element

Computes the field on elements interpolating fields in the z expression if necessary. If !element is specified and element fields appear in the z expression, those values are interpolated to the nodes first.

interfaces

Computes the field or minimum or maximum on interfaces as well as bulk. Default: true (include interfaces).

list

Returns a list of currently defined and named real data fields. This returns a full Tcl list for use with those commands that require list variables.

list.all

Returns a list of currently defined and named data fields (for example, real data and vector data). This returns a full Tcl list for use with commands that require list variables.

<material>

Specifies the material to which the command applies. Different expressions for the data field initialization in different materials can be used. See [Specifying Materials on page 18](#).

min, max

Used with the name argument. When min or max is specified, the select command returns the minimum or maximum of the field name. You can limit the query to either a specific material using <material> or a specific region using region.

name

Name of the new data field. Default: Z\_Plot\_Var. This name is used by all the commands when a plot name is not specified. This is a powerful feature, as solution fields also can be created.

node.evaluate

Computes the divergence of a vector field at a node.

permanent

Returns 1 if the data field is written into permanent storage. If not, it returns 0.

present

Returns 1 if the data field with the name defined by name exists. If it does not exist, it returns 0.

region

Name of the region. Specifies the region to which the command applies. Different expressions for the data field initialization in different regions can be used.

report.location

Works with min and max. Reports the coordinate of the minimum or maximum value of the selected field.

store

Sets the data field with the name defined by name to be written into permanent storage when a structure file is output. Default: false.

## A: Commands

select

syntax.check.value

Sets a value to be returned only during syntax-checking mode. Sometimes, the value returned by a command can cause a false syntax-check error because the value returned by the command would not be the value during the normal run mode. Setting this value avoids such problems.

value, z

Accepts an expression of data fields that are used to build a new data field. The operators \*, /, +, -, and ^ all work as expected. The vector variables are listed here. The data fields available can be listed using the list argument. In addition to the listed data fields, the x- and y-coordinates can be specified. Several functions also are available to operate on data fields:

- abs: Absolute value
- erf: Error function
- erfc: Complementary error function
- exp: Exponential
- log: Logarithm
- log10: Logarithm base 10
- sqrt: Square root

### Description

Data can be selected directly in most commands, but it is usually more effective to specify it with the select command, which allows for manipulation of data fields and also will list all currently defined data fields. The quantity can be computed on nodes (default) or elements using the element argument. In either case, if necessary, interpolation will be performed to obtain the proper value type (to obtain element values from nodal ones or vice versa).

**NOTE** The select command can be abbreviated to sel.

**NOTE** The select command always sets or retrieves data in internal units. Internal units are CGS, for example, pressure is dyn/cm<sup>2</sup>.

## Examples

Select as the plot variable the base 10 logarithm of the MyData concentration:

```
select z= log10(MyData)
```

Select as the plot variable the MyData concentration minus a constant value of  $5 \times 10^{14}$ :

```
select z= (MyData - 5.0e14)
```

Select as the plot variable the difference between the MyData profile and an analytic profile. This data field will be named MyField. The store argument indicates that the doping field must be written into any saved structure files:

```
sel z= (MyData - 1.0e18 * exp ( y * y / 1.0e-8 )) name= MyField store
```

Set the value of the data field Pressure to  $10^9$  dyn/cm<sup>2</sup> (CGS units are used internally for mechanics):

```
sel z= 1.0e9 name= Pressure store
```

Delete the MyField data field:

```
select name= MyField delete
```

Calculate the electric field in a new data field called ElectricField. The store argument ensures that the new data field is stored to disk in subsequent calls of the struct command:

```
select z= "-diff(Potential)" edge.vector store name= ElectricField
```

List all available real data fields:

```
select list
```

Calculate the total heat field in a new data field called TotalHeat:

```
select z= "grad(Temperature)" node.evaluate store name= TotalHeat
```

## See Also

All postprocessing commands

---

## Set3DDeviceMeshMode

Sets the meshing parameters for the device simulation of complex 3D structures with curved surfaces.

### Syntax

```
Set3DDeviceMeshMode
```

### Description

This command is used when remeshing for device simulation of complex 3D structures with curved surfaces. It adjusts axis-aligned meshes to be more flexible on curved surfaces in three dimensions. The Set3DDeviceMeshMode command sets the following parameters:

For device simulations requiring a box-method Delaunay mesh:

```
pdbSet Grid SnMesh DelaunayType boxmethod
```

For axis-aligned imprinting:

```
pdbSet Grid SnMesh ImprintCoplanarFacesOnly 1      ;# <boolean>
pdbSet Grid SnMesh ImprintCoplanarityAngle 179.9   ;# <degree>
pdbSet Grid SnMesh ImprintAccuracy 1e-4            ;# <um>
pdbSet Grid SnMesh ImprintCoplanarityDistance 1e-6  ;# <um>
```

For axis-aligned refinement:

```
pdbSet Grid SnMesh EdgeProximity 0.2      ;# <unitless> default 0.05
pdbSet Grid SnMesh FaceProximity 0.2      ;# <unitless> default 0.05
pdbSet Grid SnMesh CoplanarityAngle 175    ;# <degree>
pdbSet Grid SnMesh CoplanarityDistance 1e-4 ;# <um>
```

### Examples

Use this command with the DelPSC algorithm to create high-quality triangulation on curved surfaces:

```
Set3DDeviceMeshMode
pdbSet Grid SnMesh Apply.Brep.DelPSC 1
pdbSet Grid SnMesh Apply.Brep.DelPSC.Resolution 1e-2 ;# <um>
pdbSet Grid SnMesh Apply.Brep.DelPSC.Accuracy 1e-4    ;# <um>
grid remesh info= 1
```

## Limitation

Some complex structures have problematic geometric features that the DelPSC algorithm cannot tolerate. In such cases, you can use the Set3DDeviceMeshMode command without the DelPSC algorithm, for example:

```
Set3DDeviceMeshMode  
grid remesh info= 1
```

**A: Commands**Set3DMovingMeshMode

---

## Set3DMovingMeshMode

Sets the meshing parameters and relevant parameters for 3D MovingMesh applications.

### Syntax

```
Set3DMovingMeshMode <n>
```

### Arguments

<n>

Specifies the minimum feature size in micrometer. Typically, it is the smallest layer thickness of all regions.

### Description

This command simplifies the setup of moving-boundary problems by setting several parameters automatically. It checks the size of the structure and sets the appropriate parameters for the length scale. The argument <n> protects small geometric features from removal by geometry cleanup.

### Examples

Set up a 3D oxidation of a 3  $\mu\text{m}$  power structure with a 0.01  $\mu\text{m}$  thin spacer:

```
Set3DMovingMeshMode 0.01
```

Set up a 3D oxidation of a 0.1  $\mu\text{m}$  memory structure with a 0.002  $\mu\text{m}$  thin trench:

```
Set3DMovingMeshMode 0.002
```

### See Also

[MovingMesh Algorithm on page 752](#)

---

## SetAtomistic

Sets the atomistic mode as the simulation mode.

### Syntax

```
SetAtomistic
```

### Description

This command switches the simulation domain to the atomistic mode. The following commands are affected in this mode:

- deposit
- diffuse
- etch
- implant
- profile
- region
- select
- strip
- struct

If there are continuum fields, `SetAtomistic` automatically calls `PDE2KMC` to atomize the fields and to make them available as an initial state for the KMC simulation.

### See Also

[Chapter 5 on page 373](#)

**A: Commands**SetDielectricOxidationMode

---

## SetDielectricOxidationMode

Sets the oxidation mode to grow oxide with dielectric on top.

### Syntax

```
SetDielectricOxidationMode
  <Dielectric> <Oxidant>
  [Continuous | Segregation]
  [Dirichlet | MassTransfer]
```

### Arguments

Continuous, Segregation

Sets continuous boundary conditions at the dielectric–oxide interface.

Sets segregation boundary conditions at the dielectric–oxide interface.

<Dielectric>

Specifies the name of the dielectric material to grow oxide underneath.

Dirichlet, MassTransfer

Sets Dirichlet boundary conditions at the gas–dielectric interface.

Sets mass transfer boundary conditions at the gas–dielectric interface.

<Oxidant>

Specifies the name of the oxidant.

### Description

This command sets the related parameters and models for oxidation with a dielectric on top. Boundary conditions at the gas–dielectric interface and the dielectric–oxide interface default to Dirichlet and Continuous, respectively.

In addition, these settings can be changed using:

```
pdbSetString <Dielectric> <Oxidant> DielectricOxTransportBC MassTransfer
pdbSetString <Dielectric> <Oxidant> DielectricOxInterfaceBC Segregation
```

## Examples

Enable oxidation with a nitride layer on top for O<sub>2</sub> ambient, and use the mass transfer boundary condition at the gas–dielectric interface and the segregation boundary condition at the dielectric–oxide interface:

```
SetDielectricOxidationMode Nitride O2 MassTransfer Segregation
```

## See Also

[UnsetDielectricOxidationMode on page 1254](#)

## A: Commands

SetFastMode

---

# SetFastMode

Omits diffusion and Monte Carlo implantation to simulate the device geometry quickly. However, oxidation is allowed since it is considered part of structure generation.

## Syntax

```
SetFastMode
```

## Description

This command runs the simulation quickly without simulating dopants and defects. However, oxidation is simulated. This can be useful when setting up a command file to confirm quickly that the geometry is satisfactory before simulating more computationally expensive steps.

To switch off implantation, use:

```
pdbSet ImplantData NoImplant 1
```

To switch off oxidation or reaction, use:

```
pdbSet Diffuse NoDiffusionReaction 1
```

This may be useful for 3D geometry simulation.

**NOTE** The command-line option `--FastMode` (or `-f`) (see [Fast Mode on page 12](#)) for fast structure generation works slightly differently than the `SetFastMode` command. This command-line option switches off all commands that require a volume mesh such as `diffuse` (for example, `oxidation`), `kmc`, and `integrate`. This allows fast structure generation using only `etch` and `deposit` commands that modify the boundary of the structure without generating a volume mesh.

---

## SetIIIIVDiffParams

Sets the parameters and the callback procedures for diffusion in III–V materials.

### Syntax

```
SetIIIIVDiffParams <material> [<list>]
```

### Arguments

<list>

Specifies a list of dopants. If it is not specified, the necessary parameters for the material and the generic dopants are set.

<material>

Specifies the name of the III–V material.

### Description

Since there are many types of III–V material for which the parameter values are not well known for diffusion, the default values are not yet set. This command sets up the necessary parameters and the callback procedures for the diffusion simulation of the given dopants in III–V materials.

### Examples

Set up the necessary parameters and callback procedures of the dopants, Magnesium and Silicon, in the material AlGaN:

```
SetIIIIVDiffParams AlGaN {Magnesium Silicon}
```

**A: Commands**SetInterfaceInjectionLKMC

---

## SetInterfaceInjectionLKMC

Sets whether injection of point defects must be switched on during lattice kinetic Monte Carlo (LKMC) simulations.

### Syntax

```
SetInterfaceInjectionLKMC true | false
```

### Arguments

true, false

Specify whether to switch on or switch off point-defect injections during LKMC simulations.

### Description

The command specifies whether injection of point defects is switched on during the use of epitaxy models for LKMC simulations (see [Epitaxy Models Based on Atomic Bonding on page 572](#)).

### Examples

Switch on injection of point defects:

```
SetInterfaceInjectionLKMC true
```

---

## setMobilityModel

Sets the mobility model and the mobility model parameters in silicon and polysilicon for antimony, arsenic, boron, indium, and phosphorus.

### Syntax

```
setMobilityModel <c>
```

### Arguments

<c>

Specifies the name of the mobility model. Valid options are:

- Antoniadis
- Masetti
- Thurber
- Model1
- Model2
- Model3

where Model1=Antoniadis, Model2=Masetti, and Model3=Thurber.

### Description

This command sets the related parameters and switches for the mobility model given in silicon and polysilicon for antimony, arsenic, boron, indium, and phosphorus. Set values are printed in the log file.

### Examples

Set the mobility model to Masetti:

```
setMobilityModel Masetti
```

or:

```
setMobilityModel Model2
```

### See Also

[Resistivity on page 879](#)

## A: Commands

SetMoleFractionFields

---

# SetMoleFractionFields

Sets the appropriate fields of the constituent elements of an alloy material to a given material or region with given mole fractions.

## Syntax

```
SetMoleFractionFields <material_or_region> <alloy_material> <xMoleFraction>
[<yMoleFraction>]
```

## Arguments

<alloy\_material>

The name of the alloy material such as SiGe or InGaAs.

<material\_or\_region>

The name of the material or region where the fields are to be added.

<xMoleFraction>, <yMoleFraction>

Specify the required mole fraction with a value between 0 and 1 inclusively. The second mole fraction <yMoleFraction> is needed when <alloy\_material> is a quaternary material.

## Description

The constituent elements of the material (<material\_or\_region>) must be a subset of the elements of the alloy material (<alloy\_material>). Only the complementary elements of the region material are added. In other words, only the germanium field is added to a silicon material region for SiGe.

## Examples

SetMoleFractionFields is useful when you want to set the proper mole fraction after the region is formed. For example:

```
deposit SiGe thickness=0.1
```

If the deposit region is the only SiGe region in the structure, the material SiGe instead of the region name can be given:

```
SetMoleFractionFields SiGe SiGe 0.3
```

Assign Si and Ge concentrations to the region `SiGe_1` of SiGe material with  $x=0.3$ :

```
SetMoleFractionFields SiGe_1 SiGe 0.3
```

Add indium concentration to the region `GaAs_1` of GaAs material with  $x=0.47$  for  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ :

```
SetMoleFractionFields GaAs_1 InGaAs 0.47
```

Add aluminum and gallium concentrations to the material InAs region with  $x=0.2$  and  $y=0.3$  for  $\text{Al}_{0.2}\text{In}_{0.3}\text{Ga}_{0.5}\text{As}$ :

```
SetMoleFractionFields InAs AlInGaAs 0.2 0.3
```

## See Also

[GetMoleFractionFields on page 967](#)

[MoleFractionFields on page 1089](#)

**A: Commands**SetMultiphaseNickelSilicide

---

## SetMultiphaseNickelSilicide

Sets the correct parameter values for multiphase nickel silicidation.

### Syntax

```
SetMultiphaseNickelSilicide
```

### Description

This command calculates and sets the PDB parameters `Density.Grow` and `Expansion.Ratio` at the nickel–nickel silicide and nickel silicide–silicon interfaces with the parameters `MassDensity` and `Multiphase.Reaction.Rate` as well as the initial distribution values of the phases.

In addition, it executes the following commands:

```
pdbSet NickelSilicide Multiphase 1  
pdbSet Diffuse minT 100
```

The second command is required to solve equations at low temperature ( $\geq 100^{\circ}\text{C}$ ).

### See Also

[Multiphase Nickel Silicidation on page 668](#)

---

## SetPerformanceMode

Modifies the automatic time-step control method and the parameters to improve simulation time.

### Syntax

```
SetPerformanceMode [CMOS | FinFET]
```

### Arguments

CMOS, FinFET

Modifies the ILS solver settings. It uses a different setting suitable for the process type selected.

### Description

Some of the algorithms are experimental and may not be suitable for all applications. Backward compatibility may not be available from release to release, since algorithms are refined constantly.

### Examples

Change the default time-stepping scheme and the controls to allow more aggressive time-stepping:

```
SetPerformanceMode
```

Change the default time-stepping scheme, controls, and ILS solver settings for a FinFET process to allow more aggressive time-stepping:

```
SetPerformanceMode FinFET
```

## A: Commands

SetPlxList

---

# SetPlxList

Sets a list of solution and term names to be passed to the `WritePlx` command.

## Syntax

```
SetPlxList [<solution/term names>]
```

## Arguments

<solution/term names>

Defines the name list to be passed to the `WritePlx` command.

## Description

This command sets the list of fields to be saved in the next call to `WritePlx`. The list can contain solutions or term names.

## Examples

Write a .plx file with the data fields Temperature and Potential:

```
SetPlxList {Temperature Potential}  
WritePlx T_and_P.plx
```

## See Also

[WritePlx on page 1256](#)

---

## SetTDRList

Sets a list of solution or term names to be included when saving TDR format files.

### Syntax

```
SetTDRList  
  [Dopants]  
  [<solution/term names>]  
  [Solutions]
```

### Arguments

#### Dopants

Dopants include the total and active dopant concentrations. Specifying !Dopants does not save the total and active dopant concentrations, but does save NetActive (DopingConcentration). Default: true.

#### <solution/term names>

Any known fields listed on the command line are added to files saved with struct tdr=<c>.

#### Solutions

Stores all solution variables (necessary for restarting a simulation). Using !Solutions switches off all default savings (only fields specified by name will be saved to TDR files). Default: true.

### Description

This command stores solution or term names in a TDR format file.

## A: Commands

SetTemp

---

## SetTemp

Sets the temperature value.

### Syntax

```
SetTemp  
  <n> [<C> | <K>]
```

### Arguments

<n>

Specifies the temperature. Default unit: degree Celsius.

### Description

This command sets the temperature value. The value also is saved in a TDR file.

### Examples

Set the temperature to 1000°C:

```
SetTemp 1000.0
```

---

## SetTS4ImplantMode

Sets implantation-related parameters and models to match those of TSUPREM-4.

### Syntax

```
SetTS4ImplantMode [Native | Taurus]
```

### Arguments

Native

Makes simulation results close to those of the TSUPREM-4 native implanter.

Taurus

Makes simulation results close to those of the Taurus TSUPREM-4 implanter.

### Description

Sentaurus Process and TSUPREM-4 use different codes and, sometimes, have different assumptions or algorithms for analytic implantations. The SetTS4ImplantMode command tries to minimize this difference by setting appropriate switches that make Sentaurus Process simulation results as close as possible to those produced by TSUPREM-4. This includes:

- Use the beam dose.
- Switch on the `ts4.backscattering` model.
- Switch off the Sentaurus Process backscattering model.
- Switch on the `TS4FluorineMode`, which computes fluorine profiles using fluorine tables for  $\text{BF}_2$  implantation.
- In Taurus mode, also switch on the PAI model with the TSUPREM-4-compatible PAI mode.

The results may not be exactly the same due to differences in numeric methods for some cases.

---

## SetTS4MechanicsMode

Sets mechanics-related parameters and models to match those of TSUPREM-4.

### Syntax

```
SetTS4MechanicsMode [2008.09 | advanced]
```

### Arguments

2008.09

Used for backward compatibility.

advanced

Sets TSUPREM-4 advanced settings.

### Description

This command sets mechanics-related parameters and models in Sentaurus Process to match TSUPREM-4 settings. This includes:

- Viscoelastic model and parameters
- Elastic moduli
- Stress relaxation factor setting
- Stress smoothing setting
- Thermal mismatch coefficients
- Some settings for oxidation used for backward compatibility (these settings are the same as the defaults in the PDB)

The above parameters are set to match TSUPREM-4 defaults. The results may differ due to different numeric methods.

---

## SetTS4OxidationMode

Sets oxidation-related parameters and models to match those of TSUPREM-4.

### Syntax

```
SetTS4OxidationMode [2008.09 | advanced]
```

### Arguments

2008.09

Sets oxidation and mechanics parameters to Version A-2008.09 default values.

advanced

Sets parameters to TSUPREM-4 advanced settings.

### Description

This command sets oxidation-related parameters and models in Sentaurus Process to match TSUPREM-4 settings. This includes:

- Settings from SetTS4MechanicsMode
- Activation volumes of stress-dependent oxidation (SDO) reaction rate and diffusivity
- Activation volumes of stress-dependent viscosity
- Native layer thickness
- Stress-dependent oxidation flag

Because TSUPREM-4 has different values for the activation volume of stress-dependent viscosity during oxidation and nonoxidation steps, it is recommended to call SetTS4OxidationMode immediately before the oxidation step and call SetTS4MechanicsMode after it.

The above parameters are set to match TSUPREM-4 defaults. The results may not be very close due to differences in numeric methods for some cases.

---

## SetTS4PolyMode

Sets the polycrystalline model to match those of TSUPREM-4.

### Syntax

SetTS4PolyMode

### Description

This command sets the related parameters and models for the polycrystalline model in Sentaurus Process to match TSUPREM-4 settings.

---

# SheetResistance

Calculates the sheet resistance and the p-n junction depth.

## Syntax

```
SheetResistance  
[x=<n>] [y=<n>] [z=<n>]
```

## Arguments

x, y, z

Specify the cut position. For 1D simulations, no cut specification is necessary. For 2D simulations, either x or y must be specified. For 3D simulations, two axes must be specified. Default unit:  $\mu\text{m}$ .

## Description

This command calculates the sheet resistance and the p-n junction depth of a semiconductor layer in the vertical direction. It can only be used after a diffusion step.

## Examples

Calculate the sheet resistance and the p-n junction depth of a 3D structure using the cutplane  $y = 0.5 \mu\text{m}$  and  $z = -0.1 \mu\text{m}$ :

```
SheetResistance y= 0.4 z= -0.1
```

## See Also

[Chapter 14 on page 871](#)

**A: Commands**

simDelayDouble

---

## simDelayDouble

Retrieves the Tcl expression used to evaluate a double-precision simulator state variable.

### Syntax

```
simDelayDouble <c> [<c>]
```

### Arguments

<c>

This argument can be any double parameter declared in the parameter database and any double parameter declared by the user in user-defined models. In all cases, the argument must be specified with the full hierarchical path for the double parameter.

### Description

This command is very similar to the `simGetDouble` command except that the evaluation of the returned expression is delayed.

### Examples

Return `[simGetDouble Diffuse tempC]`, which is the unevaluated expression itself:

```
simDelayDouble Diffuse tempC
```

### See Also

[simGetDouble on page 1196](#)

---

## simGetBoolean

Reads a global simulator state variable.

### Syntax

```
simGetBoolean <c> [<c>]
```

### Arguments

<c>

This argument can be any double parameter declared in the parameter database and any double parameter declared by the user in user-defined models. In all cases, the argument must be specified with the full hierarchical path for the double parameter.

### Description

This command returns one of the following global simulator state variables:

- AmbientReactions
- IsEpi
- IsGrowing
- laser
- MaterialReactions

### Examples

Return true if laser annealing is switched on:

```
simGetBoolean Diffuse laser
```

## simGetDouble

Reads a double-precision simulator state variable.

### Syntax

```
simGetDouble <c> [<c>]
```

### Arguments

<c>

This argument can be any double parameter declared in the parameter database and any double parameter declared by the user in user-defined models. In all cases, the argument must be specified with the full hierarchical path for the double parameter.

### Description

This command returns a simulator set global variable. These variables are:

- EpiThick
- PH2O
- pO2
- pressure
- ramprate
- temp
- tempC
- tempK
- time
- Vt
- Vti

If the variable is not defined, it returns zero.

### Examples

Return the last diffusion temperature [K]:

```
simGetDouble Diffuse tempK
```

Return the oxygen partial pressure used during the simulation:

```
simGetDouble Diffuse pO2
```

---

## simSetBoolean

Sets a global simulator state variable.

### Syntax

```
simSetBoolean <c> [<c>] <n>
```

### Arguments

<c>

This argument can be any double parameter declared in the parameter database and any double parameter declared by the user in user-defined models. In all cases, the argument must be specified with the full hierarchical path for the double parameter.

<n>

Specifies the value of the variable.

### Description

This command sets one of the following global simulator state variables:

- AmbientReactions
- IsEpi
- IsGrowing
- laser
- MaterialReactions

**NOTE** Modifying global simulator state variables may cause errors in the simulation.

### Examples

Set the value of the global simulator state variable `laser` to true:

```
simSetBoolean Diffuse laser 1
```

## simSetDouble

Sets a double-precision simulator state variable.

### Syntax

```
simSetDouble <c> [<c>] <n>
```

### Arguments

<c>

This argument can be any double parameter declared in the parameter database and any double parameter declared by the user in user-defined models. In all cases, the argument must be specified with the full hierarchical path for the double parameter.

<n>

Specifies the value of the variable.

### Description

This command sets one of the following global double-precision simulator state variables:

- PH2O
- pO2
- temp
- tempC
- tempK
- Vti

**NOTE** Modifying global simulator state variables may cause errors in the simulation.

### Examples

Set the last diffusion temperature to 900°C :

```
simSetDouble Diffuse temp 900.0
```

---

## slice

Extracts a 1D data slice through a 2D to 3D simulation object.

### Syntax

```
slice
  [include.interfaces] [<material>]
  [mdist] [mx] [my] [mz] [name=<c>]
  [only.interfaces]
  [p1= <list>]
  [p2= <list>]
  [side=<c>] [syntax.check.value=<c>]
  [value=<n>]
  [x=<n>] [<m>|<cm>|<um>|<nm>]
  [y=<n>] [<m>|<cm>|<um>|<nm>]
  [z=<n>] [<m>|<cm>|<um>|<nm>]
```

### Arguments

include.interfaces

Includes interface values with the returned data. At an interface, the distance coordinate of the three nodes (two bulk and one interface) will be the same, and the interface value will be inserted between the two neighboring bulk values.

<material>

Specifies the material. See [Specifying Materials on page 18](#).

mdist, mx, my, mz

Changes the reporting information when interface materials are selected. The interface distance can be reported as projected along one of the three primary axes (mx, my, mz). Alternately, it can be reported as the distance along the extracted line (mdist).

name

Name of the data field. Default: z\_Plot\_Var.

only.interfaces

Returns interface values exclusively in the returned data. When specified, no bulk values are returned.

## A: Commands

slice

p1, p2

Specify the start point and endpoint for the cutline. Each argument takes a list of numeric values.

The first, second, and third values in the list are taken as the x-, y-, and z-value, respectively. The missing value will be treated as zero. These arguments allow the `slice` command to extract data along an arbitrary line. The output from the `slice` command is a list of (*distance, value*) pairs, where *distance* is measured from the `p1` point, and *value* is the extracted value of the selected quantity along the line.

**NOTE** Error messages will be generated if `p1` and `p2` are mixed with `x, y, z`, or `value`.

side

Takes the value from one of the two bulk materials consisting of the interface or ‘interface’ (literally) itself. If `side` is not specified, ‘interface’ itself is assumed. If `side` is specified as one of the bulk materials, the value of the selected quantity for the bulk material at the interface is returned. This argument is effective only if an interface material is specified.

syntax.check.value

Sets a value to be returned only during syntax-checking mode. Sometimes, the value returned by a command can cause a false syntax-check error because the value returned by the command would not be the value during the normal run mode. Setting this value avoids such problems.

value, x, y, z

Specify a cutline for up to a four-dimensional solid, so that a 2D return is provided. For 1D simulations, none of these arguments is required. For 2D simulations, one is required. For 3D simulations, two are required. These requirements are reduced by one if an interface material has been specified. The default unit for `x, y`, and `z` is  $\mu\text{m}$ .

## Description

This is an extremely powerful data analysis command. It extracts xy data along a slice through a specified material. It returns a Tcl list of coordinate–value pairs, where the coordinate is the distance [ $\mu\text{m}$ ] along the reference segment, and the value is the local value of the argument specified either with the `-name` option or, if that is not provided, in the most recent `select` command. For example:

```
select z= Boron
set sliceRet [slice y= 0.5]
foreach { x value } $sliceRet {
    LogFile "$x\t$value\n"
}
```

This command will print and send to the log file the boron profile in x-coordinate value pairs at  $y=0.5$ .

The command extracts the selected variables as a function of position along a constant line. In one dimension, the command returns the concentration versus depth, for example. It also can extract a constant contour of the data selected and returns the coordinates of the isoconcentration line.

## Examples

Return the selected variable as a function of depth at a constant lateral position of  $0.01\ \mu\text{m}$ :

```
slice silicon y= 0.01
```

Return the x- and y-positions of a contour of the selected variable at  $16.0$ :

```
slice silicon value= 16.0
```

Return the value of the selected quantity at the silicon side of the interface as a function of distance from the start of the interface:

```
slice silicon /oxide mdist side= silicon
```

Return the boron concentration along a line passing through points  $(0, 0)$  and  $(1, 2)$ :

```
slice name= Boron p1= {0 0} p2= {1. 2}
```

## See Also

[select on page 1168](#)

[tclsel on page 1222](#)

## A: Commands

smooth

---

# smooth

Smooths a set of fields.

## Syntax

```
smooth
  smooth.field= <list>
  [init=<n> [<hr>|<min>|<s>]
  [smooth.distance= {<double array>}]
```

## Arguments

init

Specifies the first time step for solving the smoothing equations. The default is 0.0001 s, which is sometimes inappropriate for defect simulations, particularly in cases of damage. Default unit: minute.

smooth.distance

Specifies the smoothing distance for each field as specified in `smooth.field`. Default: 2.0 nm.

smooth.field

List of fields to be smoothed. Any existing field can be specified.

## Description

This command smoothes a set of fields with specified smooth distances.

## Examples

Smooth the interstitial and vacancy implantation profiles with smooth distances of 2 nm and 3 nm, respectively:

```
smooth smooth.field= {Int_Implant Vac_Implant} smooth.distance= {2<nm> 3<nm>}
```

---

## solution

Obtains and sets solution parameters for generic solutions using the Alagator language.

### Syntax

```
solution
  [add]  [damp]
  [DiffStep] [GrowthStep] [Heat] [InitStep] [linear | logarithmic] [list]
  [material.list= <list>]
  [name=<c>] [needsolution] [negative]
  [nosolve | solve | ifpresent=<c>]
  [present] [reset] [smooth] [store] [unit=<c>]
```

### Arguments

add

Creates a new solution.

damp

Applies a damping algorithm to the Newton iteration.

DiffStep, GrowthStep, Heat, InitStep, smooth

Determines in which solver the solution variable will be solved:

- DiffStep variables are solved with the diffusion solver such as dopants and defects.
- GrowthStep variables are solved in the reaction step and are usually oxidants.
- Heat variables are solved during the laser annealing step.
- InitStep variables are solved during the initialization step.
- smooth variables are solved during smoothing steps (such as occurs when using the smooth command).

linear, logarithmic

Use linear or logarithmic extrapolation when extrapolating solution results for the next time step (see [math on page 1073](#)).

list

Lists all the currently defined solutions.

## A: Commands

solution

material.list

List of materials where the solution variable will be solved. If the list is empty, the solution variable will be solved only if the equations are set for a specific material.

name

The character string used for the solution. Capitalization is not ignored, for example, Potential and potential are different. Abbreviations of names are not accepted.

needsolution

Returns true if the solution must be solved.

negative

Allows the specified solution to have negative values.

nosolve, solve, ifpresent

Only one of these options can be used at a time. They control the solution status for the next command:

- nosolve means do not solve.
- solve switches on the solution status for the next command.
- ifpresent sets up a conditional solve.

If all the solutions in the specified list also are being solved, this solution is solved.

present

Returns true if the solution is defined and a data field matches the name.

reset

Allows reaction solution variables to be reset before the diffusion starts. Default: true.

store

Allows the solution command to be stored in a TDR file.

unit

Unit of the solution variable. Default: cm<sup>-3</sup>.

## Description

This command creates and modifies solution names, and sets conditions for their inclusion in the matrix assembly. Solutions also can be listed and checked.

## Examples

Create a solution named Potential and always solve for it. Allow the solution to have negative values and use damping on the Newton iteration updates:

```
solution name= Potential damp negative solve add
```

Create a solution name Vac and always solve for it. Do not use damping and do not allow values to become negative:

```
solution name= Vac !damp !negative solve add
```

Create a solution named I2 and solve for it if Int and Vac are also present and being solved:

```
solution name= I2 !damp !negative ifpresent= {Int Vac} add
```

Return a list of all solutions:

```
solution list
```

Return a Boolean true if Vac has been defined and if there is a data field with the name Vac:

```
solution name= Vac present
```

## See Also

[math on page 1073](#)  
[term on page 1232](#)

## A: Commands

sptopo

---

# sptopo

Transfers structures and dispatches commands to Sentaurus Topography.

## Syntax

```
sptopo {<Sentaurus Topography commands>}
```

## Arguments

<Sentaurus Topography commands>

Any number of Sentaurus Topography commands. Enclose the commands in a pair of braces to protect them from interpretation by the Tcl interpreter.

## Description

This command transfers the boundary representation of the current structure and dispatches the commands to Sentaurus Topography. After executing the commands in Sentaurus Topography, the modified structure is retrieved and remeshed in Sentaurus Process.

**NOTE** A license for Sentaurus Topography must be available, and a version of the Sentaurus Process binary with Sentaurus Topography included must be installed.

## Examples

Use Sentaurus Topography to deposit two layers isotropically, that is, oxide with a thickness of 0.005 μm (5 nm) and polysilicon with a thickness of 0.18 μm :

```
sptopo {  
    deposit material= Oxide thickness= 0.005  
    deposit material= PolySilicon thickness= 0.180  
}
```

## See Also

*Sentaurus™ Topography User Guide*

For 3D operations, see [topo on page 1235](#).

## stdiff

Compares the current structure with one from a TDR file.

### Syntax

```
stdiff <c>
```

### Arguments

<C>

Specifies the full path or the prefix of a TDR file. The prefix is the file name without \_fps.tdr.

### Description

This command reads the external TDR file, interpolates the data onto the current structure, compares data, and reports if data exceeds the relative error criteria (subject to the absolute error minimum value).

### Examples

Compare field values in the current structure in memory with those contained in the file n1\_fps.tdr:

```
stdiff n1_fps.tdr
```

**A: Commands**  
strain\_profile

---

## strain\_profile

Defines the strain introduced by an impurity as a piecewise linear function of the mole fraction in a given substrate.

### Syntax

```
strain_profile  
  <material> ratio= <list>  
  species=<c> strain= <list>
```

### Arguments

<material>

Substrate material where the strains are defined.

ratio

List of numeric values of the mole fraction of the species; ranges from 0 to 1.

species

Species in the substrate that cause the strain.

strain

List of numeric values of the strain caused by the specified mole fraction; ranges from 0 to 1.

### Description

The presence of certain materials such as germanium in silicon can modify the lattice spacing. This command computes strains using the impurity mole fraction.

### Examples

Define the strain profile for germanium impurity in silicon:

```
strain_profile silicon species= Germanium ratio= {0 1} strain= {0 0.0425}
```

### See Also

[transform on page 1236](#)

---

## stressdata

This command:

- Defines the intrinsic stress of materials for use in stress calculations.
- Defines boundary conditions for stress analysis.
- Reports the maximum stress values and their locations.
- Prints the anisotropic material matrix.
- Defines edge dislocation settings.

### Syntax

```
stressdata
  [<material> | region=<c>]
  [deposit.intrinsic]
  [sxxi=<n> [<atm>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
   [syyi=<n> [<atm>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
   [szzi=<n> [<atm>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
   [sxyi=<n> [<atm>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
   [syzi=<n> [<atm>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
   [szxi=<n> [<atm>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]

  [syntax.check.value]

  [base=<n> [<m>|<cm>|<um>|<nm>]
   [sxx1=<n> [<atm>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
   [syy1=<n> [<atm>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
   [szz1=<n> [<atm>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
   [sxx2=<n> [<atm>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
   [syy2=<n> [<atm>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
   [szz2=<n> [<atm>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]

  [bc.location= Left | Right | Front | Back | Bottom]
  [bc.rotation.axis= { [xa=<n>] | [ya=<n>] | [za=<n>] }]
  [bc.value= {
    [dx=<n>] | [dy=<n>] | [dz=<n>] | [pressure=<n>] |
    [pxf=<n>] | [pfy=<n>] | [pfz=<n>] |
    [rx=<n>] | [ry=<n>] | [rz=<n>] }
  [point.coord= {<n> <n> <n>}]

  [number=<n>]
  [sxx] [syy] [szz] [sxy] [syz] [szx] [hs] [pr] [ps] [vms]

  [print.anisotropic.matrix]
  [print.equiv.Poisson.matrix]
  [print.equiv.ShearMod.xy] [print.equiv.ShearMod.yz]
```

## A: Commands

stressdata

```
[print.equiv.ShearMod.zx]
[print.equiv.YoungsMod.x] [print.equiv.YoungsMod.y]
[print.equiv.YoungsMod.z]

[apply.dislocation]
[dislocation.origin= {<n> <n> <n>}]
[name=<c>]
[para.orient= {<n> <n> <n>}]
[perp.orient= {<n> <n> <n>}]
[saveTDR] [stress.relax]

[opt.maxiter=<n>] [opt.mindnrm=<n>] [opt.mindssq=<n>] [opt.tolerance=<n>]
[optimize.dislocation]
[origin.max= {<n> <n> <n>}]
[origin.min= {<n> <n> <n>}]

[resolved.shear.stress]
[slip.direction= {<n> <n> <n>}]
[slip.plane.normal= {<n> <n> <n>}]
```

## Arguments

<material>

Material in which the stress parameters are to be set.

region

Region where the stresses are to be applied.

deposit.intrinsic

Specifies that the intrinsic stress introduced during material deposition or insertion will be defined.

sxxi, syyi, szzi, sxyi, syzi, szxi

Intrinsic stresses. Default unit: dyn/cm<sup>2</sup>.

syntax.check.value

Sets a value to be returned only during syntax-checking mode. Sometimes, the value returned by a command can cause a false syntax-check error because the value returned by the command would not be the value during the normal run mode. Setting this value avoids such problems.

## Arguments: Width-Dependent Intrinsic Stress

base

Base width. Default unit:  $\mu\text{m}$ .

sxx1, syy1, szz1

Scale factors in linear width-dependent intrinsic stress. Default unit:  $\text{dyn}/\text{cm}^2$ .

sxx2, syy2, szz2

Scale factors in natural logarithmic width-dependent intrinsic stress. Default unit:  $\text{dyn}/\text{cm}^2$ .

## Arguments: Boundary Conditions

bc.location

Specifies the area where the boundary conditions are applied.

Left | Right | Front | Back | Bottom refer to the outer boundary surfaces of the simulation domain.

bc.rotation.axis

Specifies the coordinates of the point around which rotational boundary conditions or moment boundary conditions are applied. Default unit: cm.

bc.value

Specifies the boundary condition types and values. The type can be:

- $\text{dx}/\text{dy}/\text{dz}$  for the displacement rate (default unit: cm/s).
- pressure for pressure (default unit:  $\text{dyn}/\text{cm}^2$ ).
- $\text{pxf}/\text{pyf}/\text{pfz}$  for point force (default unit: dyne).
- $\text{rx}/\text{ry}/\text{rz}$  for rotational velocity (default unit: rad/s).

point.coord

Specifies the location where the point force is applied. Default unit:  $\mu\text{m}$ .

## Arguments: Maximum Stress List

number

Specifies the number of the largest stress values to report.

## A: Commands

stressdata

sxx, syy, szz, sxy, syz, szx, hs, pr, ps, vms

Specifies from which stress component (sxx, syy, szz, sxy, syz, szx) or which derived stress (vms is the von Mises stress, ps is the principal stress, hs is the hydrostatic stress, and pr is the pressure) to extract the maximum stress values. Values for stress components and principal stresses are computed at element centroid, while values for von Mises stresses, hydrostatic stresses, and pressures are computed at nodes.

**NOTE** To extract maximum principal stresses, use:

```
pdbSet Mechanics Calculate.Principal.Stress 1
```

## Arguments: Anisotropic Material Matrix

print.anisotropic.matrix

Prints the anisotropic material matrix.

print.equiv.Poisson.matrix

Prints the equivalent Poisson ratio matrix.

print.equiv.ShearMod.xy

Prints the equivalent shear modulus in the xy plane.

print.equiv.ShearMod.yz

Prints the equivalent shear modulus in the yz plane.

print.equiv.ShearMod.zx

Prints the equivalent shear modulus in the zx plane.

print.equiv.YoungsMod.x

Prints the equivalent Young's modulus in the x-direction.

print.equiv.YoungsMod.y

Prints the equivalent Young's modulus in the y-direction.

print.equiv.YoungsMod.z

Prints the equivalent Young's modulus in the z-direction.

## Arguments: Edge Dislocation

apply.dislocation

Indicates that an edge dislocation will be defined.

dislocation.origin

Specifies the location of the dislocation core.

name

Specifies the name of the edge dislocation.

para.orient

Specifies the direction of the edge dislocation.

perp.orient

Specifies the Burgers vector in the perpendicular direction to the half plane. The magnitude is the slip distance.

saveTDR

Saves the currently defined edge dislocation into a TDR file for visualization.

stress.relax

Switches on relaxation of stresses after superposing the dislocation-induced stress field.  
Default: true.

### **Arguments: Edge Dislocation–induced Strain Energy Minimization**

opt.maxiter

Specifies the maximum number of iterations allowed in the optimization loop. Default: 500.

opt.mindnrm

Specifies the change in norm of the parameter vector for convergence. Default: 5e-3.

opt.mindssq

Specifies the relative change in the sum of the squares for convergence. Default: 1e-5.

opt.tolerance

Specifies the tolerance of target errors. Default: 1e-3.

optimize.dislocation

Switches on the elastic strain energy minimization of edge dislocations defined with !apply.dislocation.

## A: Commands

stressdata

origin.max

List of numbers defining the x-, y-, and z-coordinates of the lower-right front corner of the bounding box for the location of the edge dislocation core.

origin.min

List of numbers defining the x-, y-, and z-coordinates of the upper-left back corner of the bounding box for the location of the edge dislocation core.

### Arguments: Resolved Shear Stress

resolved.shear.stress

Switches on the calculation of resolved shear stress.

slip.direction

Specifies the slip direction.

slip.plane.normal

Specifies the normal of the slip plane.

### Description

This command provides stress analysis parameters for input and output. Zero is the default value for all intrinsic stress parameters. Wherever possible, use the deposit command with specified stresses to apply intrinsic stresses.

### Examples

Set the yy component of the intrinsic stress in nitride to  $1.4 \times 10^{10}$  dyn/cm<sup>2</sup>:

```
stressdata nitride syyi= 1.4e10
```

---

## StressDependentSilicidation

Enables stress-dependent silicidation for a specified silicide.

### Syntax

```
StressDependentSilicidation <c>
```

### Arguments

<c>

Name of the silicide that will use the pressure-dependent model.

### Description

In the model, reaction rates are normal stress dependent. The diffusivity of the reactant species, silicon, (represented by the field `SiliconReact`) is pressure dependent, and the silicide is allowed to relax.

### Examples

Enable stress-dependent silicidation for nickel silicide:

```
StressDependentSilicidation NickelSilicide
```

### See Also

[Stress-Dependent Silicidation on page 671](#)

## A: Commands

strip

---

# strip

Completely removes a layer exposed to the top gas region.

## Syntax

```
strip <material> [remesh] [stress.relax]
```

## Arguments

<material>

The specified material, if exposed, is completely removed. See [Specifying Materials on page 18](#).

remesh

By default, the structure is remeshed in two dimensions after strip. Setting !remesh prevents remeshing. In three dimensions, the boundary is changed without generating a mesh, so this argument has no effect in three dimensions. Preventing remeshing can save time for very large structures.

stress.relax

Specify this option to switch on relaxation of stresses after the removal operation. Default: false.

## Description

In two dimensions, the mesh is regenerated immediately. In three dimensions, only the boundary is modified and the mesh is regenerated later when necessary.

## Examples

Remove all oxide regions exposed to the top gas region:

```
strip oxide
```

---

## struct

Writes files containing the structure or the mesh and solutions.

### Syntax

```
struct
  [Adaptive] [alt.maternames] [compress.TDR] [contacts]
  [FullD] [Gas] [interfaces]
  [mshcmd] [pdb] [pdb.only]
  [sat] [satfile=<c>] [simplify=<n>]
  [tdr=<c>] [tdr.bnd=<c>]
  [visual.1D]
  ( [x=<n>] [<m>|<cm>|<um>|<nmm>]
    [y=<n>] [<m>|<cm>|<um>|<nmm>]
    [z=<n>] [<m>|<cm>|<um>|<nmm>] )
```

### Arguments

#### Adaptive

In three dimensions, meshing is delayed until it is needed; to save a file, a mesh may need to be created. Adaptive controls whether adaptive meshing is used. The default value is the return of `pdbGet Grid Adaptive`.

#### alt.maternames

If you had chosen alternative names for materials using `mater alt.maternoame=<c>` or `region alt.maternoame=<c>`, they are written to the TDR file in addition to the Sentaurus Process material name.

For example, a Silicon region containing a high concentration of Germanium is given the alt.maternoame of SiliconGermanium automatically. When writing a TDR file, the material name of this region is SiliconGermanium, but the name Silicon is stored as well, so that when reloading the TDR file, Sentaurus Process again recognizes this as a Silicon region.

#### compress.TDR

Applies secondary compression to TDR files. Default: false.

It can also be switched on globally using the command:

```
pdbSet Compress.TDR 1
```

#### contacts

Writes contacts defined in the contact command into the boundary file. Default: true.

## A: Commands

struct

FullD

If FullD is specified, the mesh is extruded to the maximum dimension allowed in the simulation temporarily before saving the file. After saving the file, the simulation continues in the same dimension as before.

If !FullD is specified, the saved files contain mesh and data in the dimension currently used in the simulation.

**NOTE** When TDR restart files are saved, by default, no extrusion is performed.

Gas

By default, Sentaurus Process writes regions of material gas to TDR files. If !Gas is specified, regions of material gas are not saved.

interfaces

Saves interface data in TDR files. Specify !interfaces to prevent storing interface data.  
Default: true.

mshcmd

When specified with tdr or tdr.bnd, mshcmd writes a command (.cmd) file with refinement information readable by Sentaurus Mesh.

pdb

Saves pdb parameters along with the geometry and data in a TDR file.

pdb.only

Saves only pdb parameters (without geometry and data) in a TDR file.

sat

Enforces or prevents the saving of a Sentaurus Structure Editor restart file. This option works only when Sentaurus Structure Editor is switched on internally or is used as an external tool.

satfile

When using Sentaurus Structure Editor for 3D geometry-modeling steps, a Sentaurus Structure Editor restart file is saved by default. The argument satfile defines the file name. The default file extension is .sat. This argument works only when Sentaurus Structure Editor is switched on internally or is used as an external tool.

### simplify

When saving a 2D or 3D boundary in TDR files, the extracted geometry is simplified before being saved. The `simplify` argument defines the maximum deviation of the simplified boundary from the extracted geometry.

### tdr

Saves a file in TDR format. The extension `_fps.tdr` is added automatically. By default, all modifications to the parameter database are written to the TDR file to support splitting and restarting simulations.

By default, TDR files can be used to split and restart simulations. Coordinates and field values are stored with their unscaled internal values.

For information about the TDR format, refer to the *Sentaurus™ Data Explorer User Guide*.

### tdr.bnd

Writes a TDR file that contains only the boundary representation.

### visual.1D

Applies only to 1D simulations. If specified, Sentaurus Process orders the nodes when writing them in a TDR file, so that the file can be easily visualized with Sentaurus Visual.

### x, y, z

Saves a 2D cross section of a 3D structure, or a 1D cutline of any dimension structure in a TDR file. Since the file is stored in TDR format, the `tdr` argument must be used together with these arguments.

For 1D simulations, none of these arguments is required.

For 2D simulations, to save a 1D cutline, one of these arguments is required.

For 3D simulations, to save a 1D cutline, two of these arguments are needed. To save a 2D cross section, one of these arguments is required. The saved 2D cross-section TDR file can be used to restart a simulation if it is a z-cut. If you want to use other cuts for restarting simulations, rotate the structure first and then perform a z-cut.

Default unit:  $\mu\text{m}$ .

**NOTE** Only nodal data, not vector or tensor data, is stored in the saved file.

## Description

This command writes the structure and the simulation mesh and field data to one or several files. The data saved is from the current set of solution values.

## A: Commands

struct

### Examples

Write a file for device simulation (`output_fps.tdr`):

```
struct tdr= output !Gas
```

Write a TDR file with the current simulation mesh and data. By default, a restart file is written:

```
struct tdr= output
```

Write two files (`output_fps.tdr` and `output_bnd.tdr`) and apply secondary compression to the files:

```
struct tdr= output compress.TDR
```

### See Also

[contact on page 916](#)

[integrate on page 1027](#)

[math on page 1073](#)

---

## substrate\_profile

Defines the impurity profile in the substrate.

### Syntax

```
substrate_profile  
<material> species=<c>  
xcoord= <list>  
concentration= <list>
```

### Arguments

concentration

Numeric list of concentrations of the impurity at the specified xcoord.

<material>

Substrate material where the impurities will to be defined.

species

Name of the impurity.

xcoord

Numeric list of coordinates in x-direction where the concentration will be defined.

### Description

This command defines the profile of a species in a substrate in a piecewise linear manner. The piecewise linear function is given by the concentration corresponding to xcoord.

### Examples

Define the germanium profile in silicon substrate as a piecewise linear function:

```
substrate_profile Silicon species= Germanium \  
xcoord= {0 0.01 0.011 0.5 0.7 10} \  
concentration= {1e10 1e10 2e22 2e22 1e10 1e10}
```

### See Also

[transform on page 1236](#)

## A: Commands

tclsel

---

## tclsel

Selects the plot variable for the postprocessing routines.

### Syntax

```
tclsel  
[list] [<material>] [name=<c>]  
[store] [vec] [z=<c>]
```

### Arguments

list

Returns a list of currently defined and named data fields. The real data fields are listed by default. Vector data fields can be listed using vec. This returns a Tcl list for use with those commands that require list variables.

<material>

Specifies the material to which the command applies. Different expressions for the data field initialization in different materials can be used. See [Specifying Materials on page 18](#).

name

Name of the new data field. Default: z\_Plot\_Var.

This is used by all commands when a plot name is not specified. This is a powerful feature, as solution fields also can be created.

store

Controls whether the data field is written into permanent storage when a structure file is output. Default: false.

vec

Lists the vector data fields. Default: false.

z

Accepts a Tcl expression that are used to build a new data field. All valid Tcl expressions can be used in the string. Existing data fields are defined as Tcl variables, and the expression is evaluated node-by-node with the updated value of the variable. In general, this argument must be enclosed in braces, so that variable substitution is performed when the string is parsed.

## Description

This command specifies the plot variable for almost all other plot commands. It is a companion to the `select` command, but it differs from the `select` command in that it accepts any general Tcl expression. Data fields are made into Tcl variables and can be accessed with standard Tcl variable methods.

## Examples

Select as the plot variable the base 10 logarithm of the arsenic concentration:

```
tclsel z= {log10($Arsenic)}
```

Select as the plot variable the phosphorus concentration minus a constant value of  $5 \times 10^{14}$ :

```
tclsel z= {($Phosphorus - 5.0e14)}
```

Select as the plot variable the difference between the phosphorus and an analytic profile. This data field will be named `Doping`. The `store` argument indicates that the doping field must be written into any saved structure files:

```
tclsel z= {($Phosphorus - 1.0e18 * exp ( $y * $y / 1.0e-8 ))} \
name= Doping store
```

List all available real and vector data fields:

```
tclsel list vec
```

## See Also

All postprocessing commands

## A: Commands

temp\_ramp

---

## temp\_ramp

Defines a temperature profile for use with the `diffuse` command.

### Syntax

```
temp_ramp
  (clear | list | name=<c>)
  [<ambient>]
  [angles.factors= {
    [<interface_mat1>= <list>]
    [<interface_mat2>= <list>] }]
  [auto.doping= <list>]
  [coeffs= {<A0> <A1> <A2> ... <An>}]
  [crystal.rate= {"<100>"=<n> "<110>"=<n> "<111>"=<n> "<311>"=<n>
                  "<511>"=<n> "<911>"=<n> "<221>"=<n>}]
  [current.time=<n>] [<hr>|<min>|<s>]
  [delNT=<n>[<C>|<K>] | delT=<n>[<C>|<K>]]
  [density.increase= <regionName>=<n> | <material>=<n>]
  [deposit.type=<c>]
  [epi.doping= <list>] [epi.doping.final= <list>] [epi.interp= linear | log]
  [epi.layers=<i>] [epi.model=<i>]
  [epi.resist= { [<dopant1=<n>[<ohm-cm>]] [<dopant2=<n>[<ohm-cm>]] ... }]
  [epi.thickness=<n>] [<m>|<cm>|<um>|<nm>]
  [flow<ambient>=<n>] [<l/min>]
  [flows= {
    [<ambient1>=<n>] [<l/min>]
    [<ambient2>=<n>] [<l/min>]
  }]
  [gas.flow=<c>]
  [hold]
  [iiiv.epi=<c>] [ISSG]
  [last]
  [lkmc.nucleate]
  [mat.coeffs= {
    <mat1>= {<A0> <A1> <A2> ... <An>}
    <mat2>= {<A0> <A1> <A2> ... <An>}
    ...
    <matn>= {<A0> <A1> <A2> ... <An>} }]
  [p<ambient>=<n>] [<atm>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
  [partial.pressure= {
    [<ambient1>=<n>] [<atm>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
    [<ambient2>=<n>] [<atm>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
    ...}]
  [pressure=<n>] [<atm>|<GPa>|<MPa>|<KPa>|<Pa>|<dyn/cm2>]
  [ramprate=<n>] [<C/s>|<K/s>|<C/min>|<K/min>]
  [read.temp.file=<c>]
```

```
[repair]
[reset.init.time]
[sources= {<beam1> <beam2> ... <beamn>}]
[t.final=<n>] [<C>|<K>]
[temperature=<n>] [<C>|<K>] |
[time=<n>] [<hr>|<min>|<s>]
```

## Arguments

<ambient>

Shorthand specification to set the ambient partial pressure the same as the total pressure. If an ambient is specified this way, it must be the only ambient set in the temp\_ramp command.

angles.factors

Specifies interface-specific anisotropic epi growth rate factors. This argument specifies a piecewise linear growth rate factor versus angle for each growing interface (the factors must be between 0 and 1). For example, to create a 30° silicon facet and a 40° polysilicon facet, specify:

```
angles.factors= {
    EpiOnSilicon_Gas= {0.0 1.0 25.0 1.0 30 0.0}
    EpiOnPolySilicon_Gas= {0.0 1.0 35.0 1.0 40 0.0}
}
```

auto.doping

String list of species for which the auto-doping model will be switched on during epitaxial growth.

clear

Clears the global list of temperature ramps. When defining profiles, the action is to unite the new definition with any prior profiles of the same name.

coeffs

List of single-material coefficients  $A_0, A_1, \dots, A_n$  used in Fourier deposition when epi.model=1 and deposit.type=fourier.

crystal.rate

List of etching rates defined per crystallographic direction in the format:

```
{"<100>"=<dep_rate> "<110>"=<dep_rate> "<111>"=<dep_rate>
 "<311>"=<dep_rate> "<511>"=<dep_rate> "<911>"=<dep_rate>
 "<221>"=<dep_rate>}
```

## A: Commands

### temp\_ramp

used for crystallographic deposition when `epi.model=1` and `deposit.type=crystal`. Default unit:  $\mu\text{m}/\text{minute}$ .

### current.time

Returns the value of the ramp for the given time. Default unit: minute.

### delNT

Defines the maximum temperature step during a temperature ramp-down if specified. Default unit: degree Celsius. It also can be defined globally with the command:

```
pdbSet Diffuse delNT <n>
```

### deltT

Defines the maximum temperature step during a temperature ramp-up if specified. Default unit: degree Celsius. It also can be defined globally with the command:

```
pdbSet Diffuse deltT <n>
```

### density.increase

Applies densification model where the density increases in percentage. The increase value can be specified per region `<regionName>=<n>` (where `regionName` is the name of an existing region in the current structure) or per material `<material>=<n>` (where `material` is the name of a material in the current structure).

### deposit.type

When using `epi.model=1`, epitaxy is solved as a series of alternating deposition and diffuse steps. This argument specifies the deposit type, and the allowed values are:

- `isotropic` (default)
- `fourier` (in which case, either `coeffs` or `mat.coeffs` must be specified as well)
- `crystal` (in which case, `crystal.rate` must be specified as well)

### epi.doping

List of parameters where the parameter name is the name of the species to be initialized, and the value is the *initial* value. A list of fields of any name can be initialized with this argument. For solution variables, units are accepted, for example:

```
epi.doping= {boron= 1e18<cm-3> GSize= 1<nm> myfield= 1}
```

For initializing alloy fields, you can use `xMoleFraction`, or `yMoleFraction`, or both of the `MoleFractionFields` command (see [MoleFractionFields on page 1089](#)).

`epi.doping.final`

List of parameters where the parameter name is the name of the species to be initialized, and the value is the *final* value. A list of fields of any name can be initialized with this argument. For solution variables, units are accepted, for example:

```
epi.doping.final= {boron= 1e18<cm-3> GSize= 1<nm> myfield= 1}
```

For initializing alloy fields, you can use `xMoleFraction`, or `yMoleFraction`, or both of the `MoleFractionFields` command (see [MoleFractionFields on page 1089](#)).

`epi.interp`

Specifies either a linear or logarithmic gradient of doping between the values specified by `epi.doping` and `epi.doping.final`. Default: `linear`.

`epi.layers`

Number of layers of mesh lines required during epitaxial growth (for both `epi.model=0` and `epi.model=1`). The default is `-1`, which indicates that 10 layers should be used if `epi.model=1`, and 40 layers should be used if `epi.model=0`.

For `epi.model=0`, if the global parameter given by:

```
pdbSet Silicon Grid epi.perp.add.dist <n>
```

is set to a positive integer, `epi.layers` is ignored (whether set or not), and `epi.perp.add.dist` is used to determine the distance between mesh lines.

For `epi.model=1`, the number of layers is adjusted if the deposited layer thickness is less than the PDB parameter `Grid MinEpiDepositThickness` in SDE mode, or `Grid MinEpiDepositThicknessMGoals3D` in 3D MGOALS mode, or `LKMC Min.Epi.Deposit.Thickness` in LKMC epitaxial growth mode.

Both `epi.layers` and `epi.perp.add.dist` are used only during epitaxial growth. When remeshing occurs, the mesh for the entire structure, including the epitaxially grown region, is recreated without considering `epi.layers` and `epi.perp.add.dist`. Since remeshing can be triggered whenever the structure changes, even during epitaxial growth, you must define some refinement boxes in the epitaxially grown region to control the mesh there.

`epi.model`

Select the method for epitaxial growth:

- `epi.model=0` (default) applies a boundary-moving algorithm similar to oxidation.
- `epi.model=1` uses alternating doped deposition and inert annealing steps.

## A: Commands

temp\_ramp

epi.resist

List of parameters with dopant name and resistivity to calculate the background dopant concentration. If more than one dopant name appears in the list, the doping concentration is calculated individually for each dopant by ignoring the other ones.

epi.thickness

Sets the epitaxial layer thickness to be deposited. Usually, this argument must be specified for epitaxy. However, in the case of LKMC epitaxy, which is used when SetAtomistic is specified, epi.thickness can be omitted such that growth depends solely on the growth rate parameters (see [Chapter 6 on page 567](#)). Default unit:  $\mu\text{m}$ .

flow<ambient>, flows

List of gas flows in the reaction chamber. The gas flows are used to compute the partial pressures of the active ambients (those causing material growth). You can specify flows using either a parameter name composed of flow + <ambient> (for example, flowO2 and flowHCl where O2 and HCl are ambient names) or flows that takes a list of parameters with the names of the ambients, for example:

```
flows= {O2= 1.0<1/min> HCl= 1.0<1/min>}
```

[Table 81 on page 647](#) lists the available ambients, but this list can be extended by using the ambient command. When a gas flow is specified as a combination of flows (and not when using partial pressures), a complete reaction of the ambients is assumed to occur, for example,  $\text{O}_2 + 2\text{H}_2 \rightarrow 2\text{H}_2\text{O}$ . Besides gas reactions, the addition of inert gases will change the partial pressure of the material-growing ambients. For example, if the flows of only N<sub>2</sub> and O<sub>2</sub> are specified and are equal, the partial pressure of O<sub>2</sub> will be <total pressure>/2.0 where <total pressure> is given by pressure.

**NOTE** Flows and partial pressures must not be specified in the same temp\_ramp command.

gas.flow

Specifies a gas flow to be used for this temp\_ramp (must not be used with other gas\_flow arguments).

hold

During this segment of the temperature ramp, hold gives the diffuse command the opportunity to specify the time of the segment.

iiiv.epi

Specifies the name of a III–V material for epitaxial growth. An ambient must not be specified if this argument is used.

ISSG

Switches on *in situ* steam-generated (ISSG) oxidation.

last

Defines the final component of the temperature profile. There will be no more additions to the ramp.

list

Generates a list of temperature profiles. It returns a Tcl list and can be operated on as such. The default action for commands is to print the return, so if no handling is required, this prints a list of names of defined temperature profiles. If a name is specified, the temp\_ramp command only is listed along with details about the ramps.

lkmc.nucleate

Specify this option to nucleate for LKMC nonselective epitaxy on oxide or nitride.

mat.coeffs

List of multimaterial coefficients  $A_0, A_1, \dots, A_n$  used in Fourier deposition when epi.model=1 and deposit.type=fourier.

name

Name used to identify the temperature ramp. Use this name in a subsequent diffuse command.

p<ambient>, partial.pressure

List of the partial pressures of active ambients. Partial pressure specifications must not be used with flows, flow<ambient>, or pressure specifications. Partial pressures can be specified using either a parameter name composed of p + <ambient> (for example, pO<sub>2</sub> and pN<sub>2</sub>O where O<sub>2</sub> and N<sub>2</sub>O are active ambient names) or partial.pressure that takes a list of parameters with the names of the ambients, for example:

```
partial.pressure= {O2= 1.0<atm> N2O= 1.0<atm>}
```

[Table 81 on page 647](#) lists the available ambients, but this list can be extended by using the ambient command. These partial pressures are assumed to contribute to the oxidation or user-defined reaction processes. No reaction between the species is assumed. Default unit: atm.

**NOTE** Only the partial pressures of the active ambients are used directly in the oxidation reaction equations. Therefore, setting the partial pressure of inactive (in the sense that they cause a material growth reaction) ambients, such as N<sub>2</sub> and HCl, has no effect.

## A: Commands

temp\_ramp

pressure

The (total) pressure of the ambient gas. Default value and unit: 1.0 atm. This setting takes effect only if flows or flow<ambient> is defined explicitly. If gas.flow is specified, the pressure is set in the corresponding gas\_flow command.

ramprate

Temperature change during anneal. Default value and unit: 0.0°C/s .

read.temp.file

Reads a thermal profile from a file. It must not be used with any other thermal specification. To create this profile file during laser annealing, use write.temp.file of the diffuse command. The format of the file is two columns: time (in seconds) and temperature (in degree Celsius). Lines beginning with a hash (#) are ignored.

repair

In 3D MGOALS mode, small regions are removed automatically by default. Sometimes, this causes small gas bubbles in the structure or other problems. Use !repair to switch off removal of small regions.

reset.init.time

Starts each annealing step with the same initial time step.

sources

Defines deposition sources used in Fourier deposition when epi.model=1 and deposit.type=fourier.

t.final

Final temperature for a temperature ramp-up or ramp-down. It is used if ramprate is not given. The ramp time is calculated automatically. Default unit: degree Celsius.

temperature

Annealing temperature. Default unit: degree Celsius.

time

Annealing time. Default unit: minute.

## Description

This command specifies multiple-step temperature ramps and holds. It can be used to construct a complex temperature sequence to be simulated with the `diffuse` command (by specifying `temp.ramp` of the `diffuse` command).

All `gas_flow` command arguments are available with the `temp_ramp` command. [Table 81 on page 647](#) lists the available ambients and includes O<sub>2</sub>, H<sub>2</sub>O, HCl, N<sub>2</sub>, H<sub>2</sub>, Cl<sub>2</sub>, and N<sub>2</sub>O. To specify epi, an epi-type ambient must be used. By default, two are available: Epi and LTE. For more information, see [Epitaxy on page 267](#).

## Examples

Define the temperature profile named `tr1` with a temperature rate of 10 K/s:

```
temp_ramp name= tr1 temp= 20 ramprate= 10<K/s> time= 100<s>
```

## See Also

[diffuse on page 935](#)

[gas\\_flow on page 964](#)

## A: Commands

term

---

# term

Defines a new subexpression for use in the equation specification of the Alagator language.

## Syntax

```
term
  [add]  [clear]  [delete]  [eqn=<c>]  [list]
  [<material>]
  [name=<c>]  [print]  [store]
```

## Arguments

add

Creates a new term. A term with that name will be overwritten.

clear

Removes a term from the current set if the term exists. Otherwise, it clears the content of all terms.

delete

Removes a term from the current set.

eqn

The string defines the equation part of the term. The equation must conform to all the standard constraints of the Alagator language. Terms can be nested; the equation specified here can refer to other terms. Parsing of the equation is performed during diffusion, so there is no need for everything to be predefined.

list

Lists all the names of the current terms. This is returned as a Tcl list, so it can be used in conjunction with all the list functionality.

<material>

If a material is specified, the term becomes specific for this material only. This allows the same name to have different equations in different materials. See [Specifying Materials on page 18](#).

name

Reference name for the term. This name is defined and is compared to strings found in the equation parsing. Capitalization is important, and only exact matches are allowed.

**print**

Prints the equation for the term matching the name specified. If no term matches, 0.0 is returned. If the material name is not given, the first term with the matching name is returned (for example, you may obtain `VTotal` in oxide instead of silicon).

**store**

Allows the `term` command to be stored in a TDR file.

## Description

Terms are never required but can offer substantial computational benefit. Each term is evaluated only once during assembly, and the results are cached. If multiple equations refer to a term, the first equation to use it evaluates the expression and the remainder use the cached values. Terms are usually used for expressions that need to appear in several partial differential equations.

For example, a recombination term between vacancies and interstitials must appear in both the vacancy and interstitial equation. A term can be used for the recombination and can be placed in both partial differential equations. The recombination is then evaluated only once during the assembly process.

Terms can be created, searched, and printed, which allow inquiries about terms to be made in the various callback procedures. For example, the charge term in the Poisson equation can be accumulated by obtaining the current charge and adding new pieces to the term.

## Examples

Create a term named `VTotal` in silicon only. The keyword `VTotal` will be replaced with the subexpression `Vacancy+VacancyGbc`:

```
term name= VTotal add silicon eqn= "Vacancy+VacancyGbc" store
```

Create a term named `Noni` in silicon only. The equation will be the exponential of `Potential` multiplied by `$vti`. The normal rules for Tcl string variables and executions apply, so that `vti` must be a currently defined variable. The value will be replaced when the `term` command is executed:

```
term name= Noni add silicon eqn= exp(Potential*$Vti)
```

## A: Commands

### term

This is the same as the previous example. The difference is the braces around the equation, which delay variable expansion. The variable will not be expanded until the `diffuse` command is executed. This is the more normal form. You want the `Vti` variable to be replaced with the value of the current temperature of the `diffuse` command, not the temperature at the time of the `term` command execution:

```
term name= Noni add silicon eqn= {exp(Potential*$Vti)}
```

Return a list of all the current term names defined:

```
term list
```

Return the currently defined equation corresponding to the name `Charge`:

```
term name= Charge print
```

### See Also

[solution on page 1203](#)

## topo

Performs 3D etching and deposition using Sentaurus Topography 3D.

### Syntax

```
topo {<Sentaurus Topography 3D commands>}
```

### Arguments

<Sentaurus Topography 3D commands>

All arguments of the topo command are described in the *Sentaurus™ Topography 3D User Guide*.

### Description

Physical etching and deposition are available through the interface to Sentaurus Topography 3D and are executed using the topo command.

Commands entered into the topo command are passed directly to the Sentaurus Topography 3D library. The exchange of the boundary between Sentaurus Process and Sentaurus Topography 3D is handled automatically and only when required.

**NOTE** A licence for Sentaurus Topography 3D must be available, and a version of the Sentaurus Process binary with Sentaurus Topography 3D included must be installed.

## A: Commands

transform

---

# transform

Cuts, flips, reflects, rotates, stretches, or translates a structure and currently defined refinement boxes.

## Syntax

```
transform
  cut [Adaptive] [location=<n>[<m>|<cm>|<um>|<nm>] (left | right | front |
    back | up | down)]
    [max= {
      <n> [<m>|<cm>|<um>|<nm>]
      <n> [<m>|<cm>|<um>|<nm>]
      <n> [<m>|<cm>|<um>|<nm>] }
    min= {
      <n> [<m>|<cm>|<um>|<nm>]
      <n> [<m>|<cm>|<um>|<nm>]
      <n> [<m>|<cm>|<um>|<nm>] }]
    [mesh.align] [remesh] |

  flip [Adaptive] [location=<n>] [<m>|<cm>|<um>|<nm>] |

  reflect [Adaptive] [keep.original]
    (left | right | front | back) | (ymin | ymax | zmin | zmax) |

  rotate [Adaptive] [angle=<n> axis= "X" | "Y" | "Z"] |

  stretch [Adaptive] (left | right | front | back)
    [length=<n>] [<m>|<cm>|<um>|<nm>]
    [location=<n>] [<m>|<cm>|<um>|<nm>] [remesh] |

  translate= {
    <n> [<m>|<cm>|<um>|<nm>]
    <n> [<m>|<cm>|<um>|<nm>]
    <n> [<m>|<cm>|<um>|<nm>] }

  [masks]
```

## Arguments: Cut

Adaptive

If specified, Adaptive switches on adaptive meshing if remesh is given. Parameters for adaptive meshing are described in [Adaptive Mesh Refinement on page 729](#). The default is the return value of pdbGet Grid Adaptive.

`cut`

Selects the cut operation. Crops a structure using either the `max` and `min` arguments, or the `location` argument.

`location (left | right | front | back | up | down)`

Specifies the coordinate where the cut will be made. In addition, you must select one of `left`, `right`, `front`, `back`, `up`, or `down` to specify an axis-aligned cut at the coordinate given by `location`. Default value and unit:  $0.0 \mu\text{m}$ .

**NOTE** You cannot use `location` with the `max` and `min` arguments.

`max, min`

Use these two arguments to specify the new bounding box:

`max= {<maxx> <maxy> <maxz>} min= {<minx> <miny> <minz>}`

Default unit:  $\mu\text{m}$ .

**NOTE** You cannot use `max` and `min` with the `location` argument.

`mesh.align`

By default, MGOALS cuts the structure at the nearest mesh line and does not perform a remesh. If `!mesh.align` is specified, MGOALS cuts precisely at the specified coordinates and remeshes the structure.

`remesh`

Available only for two dimensions. Forces a remesh after the transformation. However, remeshing is always possible using the `grid remesh` command if required.

## Arguments: Flip

Adaptive

If specified, `Adaptive` switches on adaptive meshing. Parameters for adaptive meshing are described in [Adaptive Mesh Refinement on page 729](#). The default is the return value of `pdbGet Grid Adaptive`.

`flip`

Selects the flip operation (flips from top to bottom). See [Flip and Backside Processing on page 814](#).

## A: Commands

transform

location

Selects the x-coordinate about which the structure will be flipped. By default, the middle of the structure is chosen. Subsequent transform flip commands will, by default, use the same location for flipping whether the default is used or a chosen location is used. In three dimensions, the z-coordinate of the rotation is the middle of the structure in the z-direction. The location of the flip is also the fixed coordinate for mechanics simulations, which is otherwise at the bottom of the structure when no flip has occurred.

### Arguments: Reflection

Adaptive

If specified, Adaptive switches on adaptive meshing. Parameters for adaptive meshing are described in [Adaptive Mesh Refinement on page 729](#). The default is the return value of pdbGet Grid Adaptive.

keep.original

Retains the original structure after reflection (having both the original and the reflected structure), or stores only the reflected structure when disabled with !keep.original. Default: true.

left, right, front, back

Selects the side of the simulation domain at which the reflection is performed.

reflect

Selects the reflection operation.

ymin, ymax, zmin, zmax

Specifies the location where the reflection is performed:

- ymin is the same as left.
- ymax is the same as right.
- zmin is the same as back.
- zmax is the same as front.

### Arguments: Rotation

Adaptive

If specified, Adaptive switches on adaptive meshing. Parameters for adaptive meshing are described in [Adaptive Mesh Refinement on page 729](#). The default is the return value of pdbGet Grid Adaptive.

angle

Rotation angle. It must be one of 90, 180, or 270. Angles leading to structures having gas in a side are not allowed. This means that for axis= "Y" and axis= "Z", only 180 is allowed. For axis= "X", 90, 180, or 270 are allowed. Two-dimensional simulations are extruded into three dimensions and are then rotated.

axis

Rotation axis. It must be the x-axis, y-axis, or z-axis.

rotate

Specifies the rotation operation.

## Arguments: Stretch

adaptive

If specified, Adaptive switches on adaptive meshing. Parameters for adaptive meshing are described in [Adaptive Mesh Refinement on page 729](#). The default is the return value of `pdbGet Grid Adaptive`.

left, right, front, back

Indicates which side of the structure will be moved.

length

Length of stretching. Default value and unit: 0  $\mu\text{m}$ .

location

The y- or z-coordinate where the structure will be stretched. Default value and unit: 0  $\mu\text{m}$ .

remesh

Specifies that a remesh will be performed. Default: true.

stretch

Specifies the stretch operation.

## Arguments: Translation

translate

Translates the entire structure by specifying a translation vector:

```
translate= {<translate_x> <translate_y> <translate_z>}
```

## A: Commands

transform

Default unit:  $\mu\text{m}$ .

### Arguments: Transform Masks

masks

If this option is specified, masks will be transformed as well if present. If the `keep.original` option is specified with the `reflect` option, the reflected mask and the original mask will be combined into one mask. Otherwise, the reflected masks will replace the original ones. Default: false.

### Description

Previously, the `cut` and `clip` commands had slightly different behavior. Now, they are identical and are referred to as the `cut` command. All these transformations work in both two and three dimensions.

All these transformations, except `flip` and `stretch`, are also available in the KMC mode.

### Examples

Both commands reflect the structure and refinement boxes to the right side:

```
transform reflect right  
transform reflect ymax
```

Reflect the structure and refinement boxes to the right side and keep the reflected part only:

```
transform reflect right !keep.original
```

Stretch the structure and refinement boxes to the right side. The structure and refinement boxes left of 0.7 remain unchanged; the structure and refinement boxes to the right of 0.7 will be moved by 20 nm:

```
transform stretch location= 0.7 length= 0.02 right remesh
```

Cut the structure and refinement boxes at  $y=0.7$ . The left part will be removed without remeshing:

```
transform cut location= 0.7 left !remesh
```

Cut the structure and refinement boxes at  $x$  between  $0 \mu\text{m}$  and  $1 \mu\text{m}$ , and  $y$  between  $0 \mu\text{m}$  and  $3 \mu\text{m}$ :

```
transform cut min= {0<um> 0<um>} max= {1<um> 3<um>}
```

Shift the structure and refinement boxes up in the x-direction by 1  $\mu\text{m}$ :

```
transform translate= {-1 0 0}
```

Flip the structure and refinement boxes from top to bottom about their midpoint if it is the first flip, or store the flip location for subsequent flips:

```
transform flip
```

Rotate the structure and refinement boxes 90° in the x-axis:

```
transform rotate axis= "X" angle= 90
```

## See Also

[Handling Stress in Etching and Deposition on page 792](#)  
[mgoals on page 1083](#)

---

## transform.mask

Cuts, flips, reflects, rotates, stretches, or translates a given mask or all masks.

### Syntax

```
transform.mask
  (cut | flip | reflect | rotate | stretch)
  [angle=<n> axis= "X" | "Y" | "Z"]
  [keep.original]
  [length=<n> [<m>|<cm>|<um>|<nm>]
  [name=<c>] [name.new=<c>]
  [[location=<n> [<m>|<cm>|<um>|<nm>]
    (left | right | front | back) | (ymin | ymax | zmin | zmax)]
  [max= {
    <n> [<m>|<cm>|<um>|<nm>]
    <n> [<m>|<cm>|<um>|<nm>]
    <n> [<m>|<cm>|<um>|<nm>] }]
  min= {
    <n> [<m>|<cm>|<um>|<nm>]
    <n> [<m>|<cm>|<um>|<nm>]
    <n> [<m>|<cm>|<um>|<nm>] }]
  [translate=
    <n> [<m>|<cm>|<um>|<nm>]
    <n> [<m>|<cm>|<um>|<nm>]
    <n> [<m>|<cm>|<um>|<nm>] ]]
```

### Arguments: General

keep.original

Specifies whether to keep the original mask after a reflection operation. This option only works with the reflect option. The reflected mask and the original mask will be combined into one mask if specified. Default: true.

name

Name of the mask to apply the transformation.

name.new

Name of the transformed mask. If not specified, the transformed mask will replace the original one. If specified, a new mask will be created, and the original one will be retained.

## Arguments: Cut

cut

Crops the mask to a new bounding box (using `max` and `min`), or crops half of the mask (using either the `left`, `right`, `front`, or `back` option).

`left`, `right`, `front`, `back`

Indicates a cut at a location given by `location`, and specifies which half to remove. These options must not be used with `max` and `min`.

`location`

Specifies the y- or z-coordinate where the cut is to be performed. The `location` argument is used with `left`, `right`, `front`, or `back` to indicate which direction and side to cut. Default value and unit:  $0.0 \mu\text{m}$ .

`max`, `min`

The cut box can be specified by either:

- Both the `max` and `min` arguments:  
`max= {maxx maxy maxz} min= {minx miny minz}`
- One of `left`, `right`, `front`, or `back` to specify an axis-aligned cut at the coordinate given by the `location` argument.

Default unit:  $\mu\text{m}$ .

**NOTE** The `max` and `min` arguments must be used together. Do not use them with any of the `left`, `right`, `front`, or `back` options.

## Arguments: Flip

flip

Flips a mask (top to bottom).

`location`

Selects the x-coordinate about which the mask will be flipped. By default, the middle of the structure is chosen. Subsequent `transform flip` commands will, by default, use the same location for flipping whether the default is used or a chosen `location` is used. In three dimensions, the z-coordinate of the rotation is the middle of the structure in the z-direction.

## A: Commands

### transform.mask

#### Arguments: Reflection

left, right, front, back

Selects the side of the simulation domain at which the reflection is performed.

reflect

Indicates that a reflection will be performed.

ymin, ymax, zmin, zmax

Specify the location where the mask reflection is performed:

- ymin is the same as left.
- ymax is the same as right.
- zmin is the same as back.
- zmin is the same as front.

#### Arguments: Rotation

angle

Rotation angle.

axis

Rotation axis. It must be x, y, or z. If the rotation axis is y or z, the rotation angle must be 180.

rotate

Indicates that a rotation will be performed.

#### Arguments: Stretch

left, right, front, back

Indicates which side of the mask will be moved.

length

Length of stretching. Default value and unit: 0  $\mu\text{m}$ .

location

Specifies the y- or z-coordinate where the mask will be stretched. Default value and unit: 0  $\mu\text{m}$ .

stretch

Indicates that a stretch operation will be performed.

### Arguments: Translation

translate

Translates the mask by specifying a translation vector:

```
translate= {translate_x translate_y translate_z}
```

Default unit:  $\mu\text{m}$ .

### Description

A transformed mask is created and replaces the old one by default. The transformation applies to all existing masks, except if name is specified. In this case, a transformed mask name also can be specified using name.new. If name.new is specified, the original mask will be retained, and a new one will be created. The keep.original option can be used with reflect to combine the reflected mask and the original mask into one mask.

### Examples

Reflect all the current masks to the right side:

```
transform.mask reflect right
```

Create a new mask called smask1 by stretching the existing mask mask1 to the right side. The area left of 0.7 remains unchanged; the structure to the right of 0.7 will be moved by 20 nm:

```
transform.mask stretch location= 0.7 length= 0.02 right name= mask1 \
name.new= smask1
```

Cut all the existing masks at  $y = 0.7$ . The left part will be removed:

```
transform.mask cut location= 0.7
```

Create a new mask named new2 by copying and shifting mask2 up in the x-direction by 1  $\mu\text{m}$ :

```
transform.mask translate= {-1 0 0} name= mask2 name.new= new2
```

Rotate the mask named mask3 180° around the y-axis without changing its name:

```
transform.mask rotate axis= "Y" angle= 180 name= mask3
```

## A: Commands

transform.refinement

---

# transform.refinement

Reflects, stretches, cuts, flips, rotates, or translates a given refinement box or all refinement boxes.

## Syntax

```
transform.refinement
  (cut | flip | reflect | rotate | stretch)
  [angle=<n> axis= "X" | "Y" | "Z"]
  [keep.original]
  [length=<n>] [<m>|<cm>|<um>|<nm>]
  [name=<c>] [name.new=<c>]
  [[location=<n>] [<m>|<cm>|<um>|<nm>]
    (left | right | front | back | up | down) | (ymin | ymax | zmin | zmax)]
  [max= {
    <n> [<m>|<cm>|<um>|<nm>]
    <n> [<m>|<cm>|<um>|<nm>]
    <n> [<m>|<cm>|<um>|<nm>] }]
  [min= {
    <n> [<m>|<cm>|<um>|<nm>]
    <n> [<m>|<cm>|<um>|<nm>]
    <n> [<m>|<cm>|<um>|<nm>] }]
  [translate=
    <n> [<m>|<cm>|<um>|<nm>]
    <n> [<m>|<cm>|<um>|<nm>]
    <n> [<m>|<cm>|<um>|<nm>] ]]
```

## Arguments: General

keep.original

Specifies whether to keep the original after the transformation. When keeping the original refinement, the original is untouched, and a new one is created by transforming the original refinement. Otherwise, the refinement itself is transformed.

name

Name of the refinement to apply the transformation.

name.new

Name of the transformed refinement. If not specified, a default name is given.

## Arguments: Cut

`cut`

Crops the refinement to a new bounding box (using `max` and `min`) or crops half of it (using the `left`, `right`, `front`, `back`, `up`, or `down` arguments).

`left, right, front, back, up, down`

Indicates a cut at a location given by `location`, and specifies which half is to be removed. These arguments must not be used with `max` and `min`.

`location`

Specifies the x-, y-, or z-coordinate where the cut is to be performed. The `location` argument is used with `left`, `right`, `front`, `back`, `up`, or `down` to indicate which direction and side to cut. Default:  $0.0 \mu\text{m}$ .

`max, min`

The cut box can be specified by either:

- Both the `max` and `min` arguments:

`max= {maxx maxy maxz} min= {minx miny minz}`

- One of `left`, `right`, `front`, `back`, `up`, or `down` to specify an axis-aligned cut at the coordinate given by the `location` argument.

Default unit:  $\mu\text{m}$ .

**NOTE** The `max` and `min` arguments must be used together. Do not use them with any of the `left`, `right`, `front`, `back`, `up`, or `down` options.

## Arguments: Flip

`flip`

Flips a refinement (top to bottom).

`location`

Selects the x-coordinate about which the refinement will be flipped. By default, the middle of the structure is chosen. Subsequent `transform flip` commands will, by default, use the same location for flipping whether the default is used or a chosen `location` is used. In three dimensions, the z-coordinate of the rotation is the middle of the structure in the z-direction.

## A: Commands

transform.refinement

### Arguments: Reflection

left, right, front, back

Selects the side of the simulation domain at which the reflection is performed.

reflect

Indicates that a reflection will be performed.

ymin, ymax, zmin, zmax

Specify the location where the refinement reflection is performed:

- ymin is the same as left.
- ymax is the same as right.
- zmin is the same as back.
- zmin is the same as front.

### Arguments: Rotation

angle

Rotation angle. It must be 90, 180, or 270. Default unit: degree.

axis

Rotation axis. It must be x, y, or z.

rotate

Indicates that a rotation will be performed.

### Arguments: Stretch

left, right, front, back

Indicates which side of the refinement will be moved.

length

Length of stretching. Default value and unit: 0  $\mu\text{m}$ .

location

Specifies the y- or z-coordinate where the refinement will be stretched. Default value and unit: 0  $\mu\text{m}$ .

stretch

Indicates that a stretch operation will be performed.

### Arguments: Translation

translate

Translates the refinement by specifying a translation vector:

```
translate= {translate_x translate_y translate_z}
```

Default unit:  $\mu\text{m}$ .

### Description

A new transformed refinement box is created by default, while the old one is kept. This can be overridden with `!keep.original`. The transformation applies to all existing refinements, except if a name is specified. In this case, a transformed refinement name also can be specified by using `name.new`.

### Examples

Create a set of new refinements as reflections of all the current refinements to the right side:

```
transform.refinement reflect right
```

Create a new refinement called `sbox1` by stretching the existing refinement `box1` to the right side. The area left of 0.7 remains unchanged; the structure to the right of 0.7 will be moved by 20 nm:

```
transform.refinement stretch location= 0.7 length= 0.02 right name= box1 \
name.new= sbox1
```

Cut all the existing refinements at  $y = 0.7$ . The left part will be removed:

```
transform.refinement cut location= 0.7 !keep.original
```

Create a new refinement `new2` by copying and shifting `r1` up in the x-direction by 1  $\mu\text{m}$ :

```
transform.refinement translate= {-1 0 0} name= r1 name.new= new2
```

Rotate the refinement `refbox`  $270^\circ$  around the y-axis without changing its name:

```
transform.refinement rotate axis= "Y" angle= 270 name= refbox \
name.new= refbox !keep.original
```

**A: Commands**

transform.refinement

**See Also**

[Mesh Refinement on page 722](#)

[Handling Stress in Etching and Deposition on page 792](#)

[refinebox on page 1151](#)

[transform on page 1236](#)

---

## translate

Translates a named dataset with the specified offset.

### Syntax

```
translate
  [<material>]
  [min=<n>]
  [name=<c>]
  [offset= {<n> <n> <n>}]
```

### Arguments

<material>

If a material is specified, the dataset is translated in the specified material only. Otherwise, the dataset is translated in all materials. See [Specifying Materials on page 18](#).

min

Minimum value to fill the points with undefined value. Default: 0.0.

name

Name of a dataset. Default: z\_Plot\_Var.

offset

List of numeric values, where the first, second, and third values in the list are taken as the x-, y-, and z-value, respectively. The missing value is treated as zero.

### Description

This command spatially shifts a profile (dataset) with the specified offset. If a material is specified, the profile is shifted in the specified material only. Otherwise, the profile is shifted in all materials. When a profile is shifted, the value at some points may become undefined, in which case, these points are filled with a minimum value as specified by the min argument.

### Examples

Shift the Boron data field with a shifting vector (0.01 μm , 0.02 μm , 0.0 μm ):

```
translate name= Boron offset= {0.01 0.02}
```

---

## UnsetAtomistic

Disables the atomistic KMC diffusion model and continues the simulation using the PDE solver.

### Syntax

```
UnsetAtomistic  
[sano] [sano.list= <list>] [sano.materials= <list>]
```

### Arguments

sano

Remeshes the Sentaurus Process finite-element mesh and converts KMC particles to finite-element fields. To adaptively remesh on Sano fields and Sano-smoothed NetActive (DopingConcentration), you must specify adaptive meshing parameters *before* UnsetAtomistic.

Any adaptive criteria specified for a field that is in the Sano list will be applied to the Sano-smoothed value of the field, and any criteria specified for NetActive will be applied by default to NetActive computed from Sano-smoothed active fields. To set the list of Sano fields, use sano.list, but by default the list contains the active dopants. The field NetActive is updated automatically using Sano fields and does not need to be included explicitly.

sano.list

Lists the Sano fields. These fields are converted from KMC particle distributions using the Sano method and are used for adaptive remeshing, and subsequently converted to finite-element fields on the newly created mesh. By default, the Sano list includes all active dopants that are present. The field NetActive is updated automatically using Sano fields and does not need to be included explicitly.

sano.materials

Lists the materials in which the Sano method will be applied. By default, the list contains only Silicon because this is the only material that by default has nontrivial KMC diffusion models.

### Description

This command transfers all information into the Sentaurus Process standard mesh (by calling KMC2PDE), sets the atomistic mode to false, and deletes all atomistic-related information.

## Examples

Use the default conversion (the closest mesh point) to convert discrete particles to continuum field values:

```
UnsetAtomistic
```

Use the Sano method to convert phosphorus, arsenic, and boron particles to active concentrations:

```
UnsetAtomistic sano sano.list= {PActive AsActive BActive}
```

**A: Commands**

UnsetDielectricOxidationMode

---

## UnsetDielectricOxidationMode

Disables the oxidation mode to grow oxide with dielectric on top.

### Syntax

```
UnsetDielectricOxidationMode  
    <Dielectric> <Oxidant>
```

### Arguments

<Dielectric>

Specifies the name of the dielectric material to grow oxide underneath.

<Oxidant>

Specifies the name of the oxidant.

### Description

This command disables the dielectric oxidation mode of material <Dielectric> and ambient <Oxidant>. It deletes all the dielectric oxidation-related callback settings, the boundary conditions, and the parameter settings.

### Examples

Disable oxide growth with nitride on top of O<sub>2</sub> ambient:

```
UnsetDielectricOxidationMode Nitride O2
```

### See Also

[SetDielectricOxidationMode on page 1176](#)

---

## update\_principal\_strain

Calculates the principal strains.

### Syntax

```
update_principal_strain
```

### Description

This command calculates the first, second, and third principal strains, and stores them as the fields PrincipalStrain1, PrincipalStrain2, and PrincipalStrain3, respectively.

---

## update\_principal\_stress

Calculates the principal stresses.

### Syntax

```
update_principal_stress
```

### Description

This command calculates the first, second, and third principal stresses, and stores them as the fields PrincipalStress1, PrincipalStress2, and PrincipalStress3, respectively.

## A: Commands

### WritePlx

---

## WritePlx

Writes a 1D .plx file.

### Syntax

```
WritePlx
  <filename>
  [include.interfaces]
  [<material>]
  [only.interfaces]
  [x=<n>] [y=<n>] [z=<n>]
```

### Arguments

<filename>

Name of the output file.

**NOTE** This must be the first argument on the WritePlx command line.

include.interfaces

Includes interface values with the returned data. At an interface, the distance coordinate of the three nodes (two bulk and one interface) will be the same, and the interface value will be inserted between the two neighboring bulk values.

<material>

If a material is specified, only the plot from the given material is created. See [Specifying Materials on page 18](#).

only.interfaces

Returns interface values exclusively in the returned data. When specified, no bulk values are returned.

x, y, z

Specify the cut position. For 1D simulations, no cut specification is necessary. For 2D simulations, either x or y must be specified. For 3D simulations, two axes must be specified. It is also possible to shift .plx output files by specifying PlxShift variables. Default unit:  $\mu\text{m}$ .

## Description

This command makes a 1D profile along a given cutline and writes a .plx file of the solutions and terms given in the list provided by the SetPlxList command. If the list is not provided, only present solution names are written. If a material is specified, only data from the given material is used to create the plot.

**NOTE** The <filename> argument must be the first argument on the WritePlx command line.

## Examples

Write a 1D .plx file at the  $y = 1.5 \mu\text{m}$  cutline:

```
WritePlx 1.5.plx y= 1.5
```

Shift the axis by  $0.2 \mu\text{m}$  and write a 1D .plx file:

```
set PlxShift 0.2  
WritePlx test.plx
```

## See Also

[SetPlxList on page 1186](#)

**A: Commands**

WritePlx