

Sentaurus™ Topography 3D User Guide

Version U-2022.12, December 2022

SYNOPSYS®

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About This Guide

The Synopsys® Sentaurus™ Topography 3D tool is a three-dimensional simulator for evaluating and optimizing critical topography-processing steps such as etching and deposition.

The third-party software lp_solve 5.5, modified by Synopsys, forms part of Sentaurus Topography 3D. The modified source code (`lp_solve-5.5.zip`) is provided as part of the software package.

For additional information, see:

- The TCAD Sentaurus release notes, available on the Synopsys SolvNetPlus site (see [Accessing SolvNetPlus on page 15](#))
- Documentation available on the SolvNetPlus site

Conventions

The following conventions are used in Synopsys documentation.

Convention	Description
Bold text	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.
<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.

Customer Support

Customer support is available through the SolvNetPlus site.

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Accessing SolvNetPlus

The SolvNetPlus site includes a 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 including software downloads, documentation, and technical support.

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1. Go to <https://solvnetplus.synopsys.com>.
 - a. Enter your user name and password. (If you do not have a Synopsys user name and password, follow the instructions to register.)
-

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- Go to the Synopsys [Global Support Centers](#) site on www.synopsys.com to find email addresses and telephone numbers for Synopsys support centers throughout the world.
 - Go to the SolvNetPlus site and [open a case](#) (Synopsys user name and password required).
-

Contacting Your Local TCAD Support Team Directly

Send an email 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
-

Statement on Inclusivity and Diversity

Synopsys is committed to creating an inclusive environment where every employee, customer, and partner feels welcomed. We are reviewing and removing exclusionary language from our products and supporting customer-facing collateral. Our effort also

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includes internal initiatives to remove biased language from our engineering and working environment, including terms that are embedded in our software and IPs. At the same time, we are working to ensure that our web content and software applications are usable to people of varying abilities. You may still find examples of non-inclusive language in our software or documentation as our IPs implement industry-standard specifications that are currently under review to remove exclusionary language.

1

Introduction to Sentaurus Topography 3D

This chapter introduces the functionality of the Sentaurus Topography 3D tool, the required input files, and the generated output files.

Sentaurus Topography 3D is a three-dimensional simulator for evaluating and optimizing critical topography-processing steps such as etching and deposition. Two- and three-dimensional structures composed of an arbitrary number of different materials can be handled.

The initial structure can either be created using simple geometric etching and deposition operations, or be read in from TDR files. The resulting structures can be saved in different TDR file formats and can be used for further processing.

Starting Sentaurus Topography 3D

Sentaurus Topography 3D can be invoked and used in different modes.

From Sentaurus Workbench

Sentaurus Topography 3D is fully integrated in Sentaurus Workbench. On the command line, enter the following command to start Sentaurus Workbench:

```
swb
```

Inside Sentaurus Workbench, you can add Sentaurus Topography 3D to any process flow.

From the Command Line

You can start Sentaurus Topography 3D directly from the command line by specifying:

```
sptopo3d [<options>] commandfile.cmd
```

Chapter 1: Introduction to Sentaurus Topography 3D

Starting Sentaurus Topography 3D

where `commandfile.cmd` is a file containing all the commands for a simulation. See [Chapter 6 on page 137](#) for detailed descriptions of commands.

Table 1 Command-line options for Sentaurus Topography 3D

Option	Description
<code>--keep_parallel_licenses</code>	If you specify this option, then parallel licenses remain checked out after a command using them has been executed. Specifying the <code>keep_parallel_licenses</code> parameter of the <code>let</code> command has no effect when this command-line option is used (see let on page 501). Note: This option is useful to globally change whether parallel licenses must remain checked out after a command using them has been executed without modifying command files. For example, it can be used in the tool databases of Sentaurus Workbench at the global, site, or user level as follows: <pre>set WB_tool(sptopo3d,cmd_line) "-- keep_parallel_licenses n@node@_t3d.cmd"</pre>
	See <i>Sentaurus™ Workbench User Guide</i> , Tool Databases.
<code>--max_threads <i></code>	Sets the maximum number of threads per process to be used to execute the commands specified in the command file. Its value must be an integer greater than zero. If the number of threads specified by either the <code>num_threads</code> parameter of the <code>let</code> command or the <code>--threads</code> option exceeds the value of <code>--max_threads</code> , then the number of used threads is set equal to the value of <code>--max_threads</code> (see let on page 501 and the <code>--threads</code> entry in this table). If you do not specify this option, no limit on the number of threads per process is enforced.
<code>--mpi-file <c></code>	Sets the name of the file containing a list of hosts where you can run the processes to be used to execute the commands specified in the command file. For details, see <i>TCAD Parallelization Environment Setup User Guide</i> , Creating the MPI Host File. You can specify this option only when the number of processes set by <code>--processes</code> is greater than 1. If you do not specify this option, all processes run on the host where Sentaurus Topography 3D is started.
<code>--no_html_report</code>	If you specify this option, then the <code>etch</code> command does not produce a report (HTML file) of a particle Monte Carlo (PMC) simulation.

Chapter 1: Introduction to Sentaurus Topography 3D

Starting Sentaurus Topography 3D

Table 1 Command-line options for Sentaurus Topography 3D (Continued)

Option	Description
--no_intermediate_extraction	If you specify this option, then the <code>deposit</code> and <code>etch</code> commands do not execute intermediate extractions and do not produce output files for such extractions.
--no_intermediate_plot	If you specify this option, then the <code>deposit</code> and <code>etch</code> commands do not calculate intermediate plots and do not produce output files for such plots.
--no_save	If you specify this option, then the <code>save</code> command does not produce output files.
--processes <i>	Sets the number of processes to be used for executing the commands specified in the command file. Its value must be an integer greater than zero. If you do not specify this option, one process is used.
--ssh-check yes no	Specifies whether to test all hosts used by Sentaurus Topography 3D for a silent SSH login before Sentaurus Topography 3D starts. If you do not specify this option, then all hosts are tested. You can specify this option only when the number of processes set by <code>--processes</code> is greater than 1.
--threads <i>	Sets the maximum number of threads per process to be used to execute the commands that support shared-memory parallelization, specified in the command file. Its value must be an integer greater than zero. Specifying the <code>parallel</code> and <code>num_threads</code> parameters of the <code>let</code> command has no effect when this command-line option is used (see let on page 501).
--use_datex true false	When using material names defined in the <code>datexcodes.txt</code> file, the default behavior (<code>--use_datex true</code>) is that these names are translated to the canonical name for the specified material. Specify <code>--use_datex false</code> to deactivate the use of DATEX material aliases (see Material Names and Aliases on page 37).

Examples

Start Sentaurus Topography 3D on the local host using one process with four threads:

```
sptopo3d --threads 4 commandfile.cmd
```

Chapter 1: Introduction to Sentaurus Topography 3D

Input Files

Start Sentaurus Topography 3D using two processes on the hosts listed in the file `hostfile`, using 8 threads for each process:

```
sptopo3d --mpi-file hostfile --processes 2 --threads 8 commandfile.cmd
```

Start Sentaurus Topography 3D on the local host using one process with four threads, and specify globally that the `deposit` and `etch` commands do not calculate intermediate plots and do not produce output for such plots:

```
sptopo3d --threads 4 --no_intermediate_plot commandfile.cmd
```

Input Files

Sentaurus Topography 3D uses the following input files depending on the initial information available to start a simulation.

Command File

The command file is a text file that contains a sequence of commands that direct the simulation (see [Chapter 6 on page 137](#)). The command file can also contain Tcl commands.

TDR File

The initial structure for a simulation can be read from a TDR file containing a 2D or 3D boundary, or a 3D GC structure. The 3D boundary must have a rectangular base normal to the positive z-axis.

PMC File

The initial structure for a particle Monte Carlo (PMC) simulation can be read from a PMC file.

Output Files

The names of output files created by Sentaurus Topography 3D follow a naming convention. The base name of the output files is defined by the base name of the command file. Different extensions are used, depending on the type of the output file.

Standard Output and Log File

All the commands specified by the input file as well as the messages and output indicating the progress of Sentaurus Topography 3D are, by default, displayed on-screen. Any error or warning condition encountered is also displayed.

The log file has the extension `.log` and contains the same information as the standard output. The file should be examined after completion of a Sentaurus Topography 3D simulation.

TDR Files

Different TDR file formats can be used to save information about structures modified by a Sentaurus Topography 3D simulation. You can use the `save` command (see [save on page 521](#)), for example, to:

- Save structure boundary information at any stage of a simulation
- Save the resulting structure of a simulation that used the particle Monte Carlo method

Furthermore, you can use the `extract` command to save 1D and 2D geometric information from a structure into TDR files (see [extract on page 437](#)).

PMC File

A PMC structure can be saved to a PMC file, which can be subsequently read in to define the initial structure of a new PMC simulation.

TCAD Sentaurus Tutorial: Simulation Projects

The TCAD Sentaurus Tutorial provides projects demonstrating the capabilities of Sentaurus Topography 3D.

To access the TCAD Sentaurus Tutorial:

1. Open Sentaurus Workbench by entering the following on the command line: `swb`
2. From the menu bar of Sentaurus Workbench, choose **Help > Training** or click  on the toolbar.

Chapter 1: Introduction to Sentaurus Topography 3D

TCAD Sentaurus Tutorial: Simulation Projects

Alternatively, to access the TCAD Sentaurus Tutorial:

1. Go to the \$STROOT/tcad/current/Sentaurus_Training directory.

The STROOT environment variable indicates where the Synopsys TCAD distribution has been installed.

2. Open the index.html file in your browser.

2

Simulation Details

This chapter provides details about simulations performed using Sentaurus Topography 3D.

Sentaurus Topography 3D Computational Model

Sentaurus Topography 3D simulates deposition, etching, and simultaneous etching and deposition processes using physical and geometric models. Except for the spin-on-glass deposition model, two simulation methods are used to implement the physical models: the level-set method and the particle Monte Carlo (PMC) method.

Some physical models can be run only using the level-set method and others can be run only using the PMC method. To the former class belong the following models:

- Rate formula module (RFM)-based models (see [Chapter 8 on page 564](#)).
- Built-in models:
 - Etching and simultaneous etching and deposition models: `crystal`, `dry`, `etchdepo`, `etchdepo2`, `hdp`, `ion_enhanced`, `ionmill`, `rie`, `rie2`, `simple`, and `wet`
 - Deposition models: `ald`, `crystal`, `electrodeposition`, `electroplating`, `hdp`, `hdp2`, `lpcvd`, `pecvd`, `pvd`, and `simple`

To the latter class belong the reaction models, that is, those defined in terms of reactions rather than rate formulas (see [add_reaction on page 182](#) and [define_model on page 289](#)).

For the spin-on-glass deposition model (named `spin_on`), the surface profile evolution is determined by solving a partial differential equation describing the motion of a fluid driven by surface tension, centrifugal forces, and evaporation (see [Spin-on-Glass Deposition Model on page 81](#)).

All Sentaurus Topography 3D models take as input the structure at the beginning of the simulated process step and produce as output the structure resulting from the simulated process step.

Chapter 2: Simulation Details

Sentaurus Topography 3D Computational Model

The internal representation of the output structure depends on the model used and might differ from the internal representation of the input structure. Sentaurus Topography 3D uses the following main internal structure representations:

- Boundary representation
- Volumetric representation

The output of geometric models and models based on the level-set method is stored internally using the boundary representation. In contrast, the output of PMC-based models is stored internally using the volumetric representation.

In this manual, for brevity, structures stored internally using the boundary representation are referred to as *boundary structures* and structures stored internally using the volumetric representation are referred to as *PMC structures*.

Computational Model When Using the Level-Set Method

When using the level-set method to simulate a model, the exposed surface (see [Boundary Types on page 31](#)) is discretized into a set of surface elements of finite extents, and the processing time is divided into discrete time steps.

At each time step, the velocity at each surface element is determined according to the processing conditions, and the surface is updated. The velocity is computed using the *rate formula*, which is specific to each model, because it expresses with a mathematical relation the deposition or etching mechanisms relevant to the modeled process.

For example, the rate formula of the LPCVD model ([Equation 16 on page 65](#)) states that the deposition rate at any surface point is proportional to the number of neutral particles hitting the surface per unit time and area, including both those reaching the surface directly from the reactor and those that are reemitted from other surface points.

At each time step, all the quantities involved in the rate formula are computed, and the velocities are determined accordingly at each surface point. Among such quantities, a crucial role is usually played by the number of particles hitting the surface per unit time and area, as described for the LPCVD model.

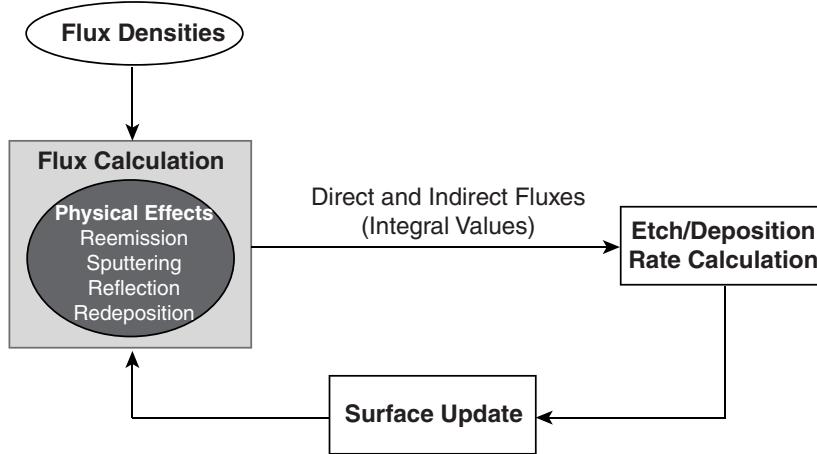
For level set-based models, Sentaurus Topography 3D uses the concept of *flux* to model the flow of particles and their interactions with the surface. In this context, a flux denotes an abstract continuum representation of one or more chemical species having a similar role in the modeled process. Therefore, *abstract* means that different chemical species (which are really involved in the process) can be included in the simulation as a single flux.

The term *continuum* refers to the fact that species are not modeled as sets of discrete particles, but by a continuum flow that is characterized by statistical properties such as the angular distribution or the energy distribution. On this basis, a flux can be considered a continuum of abstract particles.

Chapter 2: Simulation Details

Sentaurus Topography 3D Computational Model

Figure 1 Conceptual model of Sentaurus Topography 3D when using the level-set method



As explained in [Modeling Fluxes and Related Physical Effects on page 44](#), there are different kinds of flux for level set-based models:

- Fluxes with isotropic angular distribution, which are called neutrals
- Fluxes with an anisotropic angular distribution, which are called ion fluxes

The different interactions between a flux and the surface are *physical effects*. Sentaurus Topography 3D supports the physical effects of reemission for neutral fluxes, and reflection, sputtering, and deposition of sputtered material for ion fluxes.

As mentioned, a flux provides a continuum representation of a set of species. More precisely, every flux is characterized by its flux density, which describes the statistical distribution of the velocities of the particles as emitted from their source.

The scalar quantity called the *direct flux* denotes the integrated flux density on a point of the surface. The direct flux is the integral of the flux density over the visible range of the surface point, or the number of particles per unit area and time that reaches the surface at this point before having interacted with the surface.

Note:

When using the level-set method, flux densities are always normalized such that the direct flux is equal to 1 on a completely visible flat surface.

A secondary flux that results from an interaction with the surface is referred to as an *indirect flux*. For example, the number of sputtered particles per unit area and time is referred to as the *sputtered flux*.

Consequently, for each flux, there is one direct flux and possibly several indirect fluxes, according to the modeled physical effects. All these fluxes can be used in the rate formula.

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Discretization Size and Accuracy

At each time step, all the direct and indirect fluxes involved in the rate formula are computed at each surface point. The computation of all the direct and indirect fluxes requires knowledge about the flux densities and the shape of the surface. Accordingly, when using the level-set method, the computational flow of Sentaurus Topography 3D can be described as a loop over the following three stages:

1. If the model depends on fluxes, compute the direct flux and all indirect fluxes for each flux at each surface point.
2. Compute the velocity at each surface point according to the rate formula.
3. Move the surface according to the velocities provided by the rate formula.

Computational Model When Using the PMC Method

The PMC method uses a stochastic approach to compute the time evolution of a structure. You define interactions between the plasma species and the wafer species in terms of surface reactions (see [add_reaction on page 182](#), [add_source_species on page 203](#), and [define_model on page 289](#)).

Computational Model for Spin-on-Glass Deposition

The time evolution of the film profile is determined by solving a partial differential equation describing the motion of a fluid driven by surface tension, centrifugal forces, and evaporation (see [Spin-on-Glass Deposition Model on page 81](#)).

The processing time is divided into discrete time steps, and the surface is sampled at a set of points. At each time step, the height of the film is computed at each sampling point, and the film profile is updated until the total process time is reached.

Discretization Size and Accuracy

Numeric simulation methods, in general, only produce approximations to the exact results. Usually, the quality of the approximation can be improved by increasing the computational effort. For the level-set method and the method used to solve the spin-on-glass deposition model, the required memory and CPU time are determined mainly by the spatial and time discretization.

For the PMC method, the required memory and the CPU time depend mainly on the spatial discretization, the number of simulated particles coming from the reactor, and the number of simulated reactions.

In Sentaurus Topography 3D, the `spacing` parameter of the `deposit` and `etch` commands sets the grid discretization used to compute the structure evolution (see [deposit on](#)

Chapter 2: Simulation Details

Discretization Size and Accuracy

[page 375](#) and [etch on page 399](#)). The `flux` parameter of the `define_species_distribution` command (see [define_species_distribution on page 337](#)) as well as the parameter `time` of the `etch` command (see [etch on page 399](#)) determine the number of simulated particles.

Decreasing the size of the spatial discretization increases the required memory and the CPU time because there are more grid points to store and process. When using the level-set method, due to the Courant–Friedrichs–Lewy (CFL) condition [1], the maximum time-step size must be reduced. This causes a further increase of the CPU time.

Usually when setting up an etching or a deposition simulation, it is necessary to find a compromise between the required accuracy and the limited available computational resources. A good understanding of the relationship between the discretization sizes and the resulting accuracy is important not only when setting up a simulation, but also when interpreting the results of a simulation.

You can set the spatial discretization for each coordinate axis of the computational grid. For models using the level sets, the spatial discretization along each dimension of the structure can be set. For the spin-on-glass deposition model, since the vertical dimension does not need to be discretized, only the spatial discretizations along dimensions orthogonal to the vertical can be set. You might choose the discretization in a certain direction to be much coarser than for the other directions to reduce simulation time. This is not recommended, however, for various implementation-specific reasons. It is recommended that the discretization for all axes does not vary by orders of magnitude. It has been found that a factor of three between the discretization of the axes produces good results. For models using the PMC method, the spatial discretization along all dimensions must be the same (see [deposit on page 375](#) and [etch on page 399](#)).

Discretization Size and Accuracy When Using the Level-Set Method

In general, the spatial accuracy that can be achieved when using the level-set method is of the order of the spatial discretization. Therefore, you must decide which features of the input structure and the expected output structure are important and choose the spatial discretization accordingly.

For models using the level sets, subresolution accuracy can be achieved in those parts of the simulation domain where the surface shows little variation. For example, when using a deposition model for which the rate does not depend on any property of the surface, the thickness of a deposited layer can be determined with higher accuracy than the spatial discretization size in those areas of the surface that are at a distance from the corners of the surface.

For etching, the situation is more complicated, and some additional considerations must be taken into account. Generally, several materials are etched simultaneously with different etching rates. Sentaurus Topography 3D determines the material-dependent etching rate on the exposed surface.

Chapter 2: Simulation Details

Simulation Flow

To underetch masking materials properly and to avoid certain artifacts, special treatment is necessary at the interface of two different materials. At an interface, the highest etching rate of the materials next to the interface is used. This can lead to problems with very thin layers for which the etching rate is lower than for the neighboring materials, because these thin layers can be etched away in one time-step. To avoid this, it is suggested that the spatial discretization is set to slightly less than the thickness of the thin layer.

As described in [Computational Model When Using the Level-Set Method on page 24](#), at each time step, the exposed surface (see [Boundary Types on page 31](#)) of the processed structure is discretized into surface elements of finite extents, whose sizes depend on the level-set grid spacing.

To determine the values of the material-dependent parameters involved in the rate formulas of etching models and simultaneous etching and deposition models, it is necessary to compute the material or the materials through which each element of the exposed surface passes.

Since the surface discretization depends on the level-set grid, but the material information comes from the input structure, it is possible that some surface elements pass through multiple materials of the structure. This might happen, for example, when an interface between two materials of a structure is not aligned with the level-set grid.

In such cases, the default behavior of Sentaurus Topography 3D is to assign to each surface element the material in which its centroid is contained. When better accuracy is needed, you can change this behavior by setting `region_query_accuracy=subresolution` in the `etch` command (see [etch on page 399](#)). When `region_query_accuracy=subresolution`, the etching or deposition rate of each surface element is computed by taking into account all materials through which a surface element passes.

Simulation Flow

In Sentaurus Topography 3D, independently of the used numeric method, the simulation of a physical process requires:

- A model describing the process of interest
- A structure to be processed

When a process step simulation is complete, you can write the resulting structure to a TDR file (see [Output Files on page 20](#) and [save on page 521](#)) or perform measurements on it using the `extract` command (see [extract on page 437](#)).

A model and its parameter values are specified by defining a machine, as detailed in [Machines on page 29](#). A machine can be applied to simulate a process running on any structure.

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Simulation Flow

You can create a structure by either using Sentaurus Topography 3D commands or loading a TDR file (see [Initial Structure Generation on page 29](#) for an overview of the commands available to define the initial structure of a simulation and the related concepts).

Machines

Sentaurus Topography 3D can simulate different topography processes: deposition, etching, and lithography. Each process is represented by a machine that groups all of the parameters necessary to perform a simulation (see [define_deposit_machine on page 220](#), [define_etch_machine on page 242](#), or [define_litho_machine on page 280](#)).

Machines must be defined before their use, and a unique name for a given machine type (either deposition, etch, or lithography) must be assigned. When only one machine is defined, the name definition can be omitted and the simulator assigns the default machine name. If more than one machine of the same type is needed, a unique name must be set for each of the defined machines.

The definition of different machines with a corresponding unique name allows the creation of a machine library. A machine defined in such a library can be referenced at any time during the simulation.

Initial Structure Generation

The input structure to be processed in Sentaurus Topography 3D can be obtained in either of the following ways:

- Load a TDR boundary file, for example, `define_structure_file=input.tdr`.
- Create a structure directly in Sentaurus Topography 3D, using a combination of simple geometric etch and deposition steps.

The second option is useful to create simple input structures without using external tools, as discussed in the next sections.

Creating the Initial Structure

When a structure is created with Sentaurus Topography 3D, an initial cuboid structure must be defined. This structure constitutes the base for further etch or deposition processes. The following command creates a unit cube made of silicon (see [define_structure on page 360](#)):

```
define_structure material=Silicon point_min={0 0 0} point_max={1 1 1}
```

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Simulation Flow

Modifying the Initial Structure

The initial cuboid region can be modified either by adding materials using the `deposit` command or by removing parts of the structure using the `etch` command.

The following commands etch a rectangular trench out of the initial cuboid defined above:

```
define_shape type=cube point_min={0 0.3 0.5} point_max={1 0.7 1.0} \
    name=etch_shape
etch shape=etch_shape
```

The first command defines a cuboid shape that overlaps the original unit cube (see [define_shape on page 313](#)). The second command uses the defined cube `etch_shape` to remove material from the unit cube (see [etch on page 399](#)).

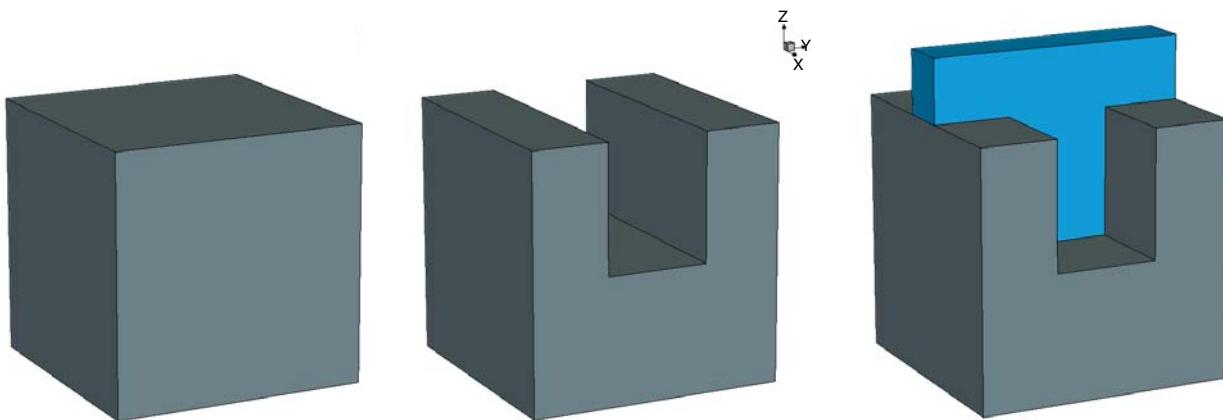
Similarly, it is possible to deposit a cuboid region:

```
define_shape type=cube point_min={0.4 0 0.5} point_max={0.6 1 1.25} \
    name=depo_shape
deposit shape=depo_shape material=Tungsten
```

The above commands define a cube, which is deposited over the trench created earlier. In the `deposit` command, the deposited material must be specified (see [deposit on page 375](#)). Parts of `depo_shape` that overlap the existing structure will not be added.

The structure that has been created could now be saved for visualization by using the command `save` (see [save on page 521](#)). It can also be used as the initial structure for physics-based etch or deposition steps. [Figure 2](#) shows the results of the commands in this section.

Figure 2 *Initial structure generation: (left) initial cuboid structure, (middle) trench etched from the initial structure, and (right) cuboid deposited on the trench*



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Simulation Flow

Note:

When using level set-based models or the spin-on-glass deposition model, Sentaurus Topography 3D does not require the presence of any gas region on top of the initial structure. However, if the initial structure contains gas regions, gas will be present also in the final structure.

When using a reaction model based on the PMC method, where deposition is allowed, the computational domain must be sufficiently large to contain also the material that will be deposited during the simulation (see [Boundary Types on page 31](#)). This goal can be achieved by adding a gas region on top of the initial structure.

A gas region can be added to an existing structure using the `fill` command (see [fill on page 477](#)). This feature is useful also if a structure produced by Sentaurus Topography 3D must be read by other tools that require the presence of gas on top of their initial structure.

Boundary Types

As described in [Input Files on page 20](#), Sentaurus Topography 3D loads two- or three-dimensional TDR boundary files containing all the geometric and material information of the structure that must be processed.

[Figure 3 on page 32](#) (a) shows a cross section of a typical 3D structure that can be used as the *initial structure* of a simulation. The computational domain is defined as the minimum bounding box that contains the structure (see [Figure 3](#) (b)).

The upper part of the surface of the structure is called the *exposed surface* (see [Figure 3](#) (c)). When using the level-set method or the spin-on-glass deposition model, the exposed surface evolves until the end of the simulation when a final profile of it is obtained (see [Figure 3](#) (d)).

At the end of the simulation, the final exposed surface can be combined with the lateral and the bottom planes of the computational domain, resulting in the *closed surface* (see [Figure 3](#) (e)).

Using Boolean operations, a boundary representation of the final structure, hereafter referred to as the *final boundary structure* (see [Figure 3](#) (f)), which includes all material information, can be created from the initial structure (see [Figure 3](#) (a)) and the closed surface (see [Figure 3](#) (e)).

The boundary data structures – exposed surface, closed surface, and final boundary structure – can be saved in a TDR boundary file using the `save` command (see [save on page 521](#)).

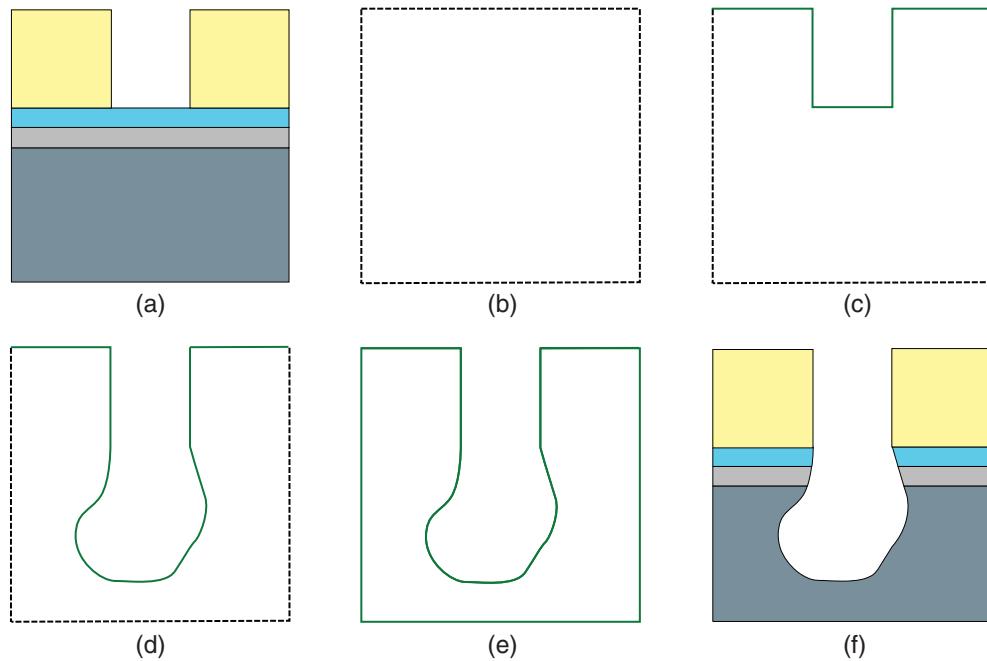
The final boundary structure contains much more information than the exposed and closed surfaces, but the Boolean operations can be computationally expensive.

Chapter 2: Simulation Details

Simulating Process Steps on 2D and 3D Structures

The final structure is necessary and must be saved when transferring the simulation results to another TCAD Sentaurus tool (for example, Sentaurus Process).

Figure 3 Cross section of a 3D structure: (a) initial structure, (b) initial computational domain, (c) initial exposed surface, (d) final exposed surface, (e) final closed surface, and (f) final structure



Simulating Process Steps on 2D and 3D Structures

When using a level set-based model or the spin-on-glass deposition model, Sentaurus Topography 3D can simulate process steps on both two-dimensional (2D) and three-dimensional (3D) structures. Two-dimensional and 3D structures can be simulated using the same physical models, with consistent results. When using the PMC simulation method, only process steps on 3D structures can be simulated.

Simulating 2D cuts of 3D structures typically is orders of magnitude faster than a full 3D simulation. Flux integration for 2D structures is performed using the radiosity method. No Monte Carlo implementation is provided.

For a full list of limitations, see [Limitations When Processing 2D Structures on page 34](#) and [Chapter 11 on page 592](#).

Sentaurus Topography 3D provides a command language that is mostly independent of the dimension of the structure to simulate.

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Simulating Process Steps on 2D and 3D Structures

A structure is defined by the `define_structure` command (see [define_structure on page 360](#)), and there are two use cases:

- `define_structure file=<c> [name=<c>]`

Sentaurus Topography 3D reads the file specified by the parameter `file`. The last 2D or 3D TDR boundary contained in that file is used to create a structure with the name specified by the parameter `name` or with the default name `default_structure`.

- `define_structure material=<c> point_max=<v> point_min=<v> [name=<c>]`

Sentaurus Topography 3D creates a structure – a cube or a rectangle – depending on the length of the vectors used for the parameters `point_min` and `point_max`, with the name specified by the parameter `name` or with the default name `default_structure`.

Any other command either refers to an already defined structure (through its `structure` parameter) or does not operate on any structure. In this way, you can mix 2D and 3D simulations in the same input file, as shown in the following example:

```
# Define a 3D structure called 'structure_3d'. The dimension of the
# created structure is determined by the size of the 'point_min'
# and 'point_max' parameter values.
define_structure name=structure_3d material=Silicon \
    point_min={0 0 0} point_max={1 1 1}

# Define a 2D structure called 'structure_2d'. The dimension of the
# created structure is determined by the size of the 'point_min' and
# 'point_max' parameter values.
define_structure name=structure_2d material=Oxide \
    point_min={0 0} point_max={1 1}

# Define a deposition machine. The 'define_deposit_machine' command
# does not operate on any structure and the machine it defines can
# be used with both 2D and 3D structures.
define_deposit_machine anisotropy=0.8 curvature=0 material=Nitride \
    model=simple rate=1

# Simulate a deposition process for the 2D structure 'structure_2d'
# and save the result. Because the referred structure is 2D, a 2D
# simulation will be run.
deposit spacing=0.1 structure=structure_2d time=1

# Save the result of the deposition step for structure 'structure_2d'.
save structure=structure_2d

# Simulate a deposition process for the 3D structure 'structure_3d'
# and save the result. This command looks exactly like the one above.
# It only refers to a different structure. Because the referred
# structure is 3D, a 3D simulation will be run.
deposit spacing=0.1 structure=structure_3d time=1

# Save the result of the deposition step for structure 'structure_3d'.
```

Chapter 2: Simulation Details

Simulating Process Steps on 2D and 3D Structures

```
save structure=structure_3d

# Simulate another deposition process for the 3D structure 'structure_3d'
# and save the result. Because a discretization that is not uniform
# across the coordinate directions is specified, the length of the value
# of the 'spacing' parameter must match the dimension of the structure
# this command operates on. If the structure had dimension 2, an error
# will be issued by the 'deposit' command.
deposit spacing={0.1 0.5 0.025} structure=structure_3d time=1

# Save the result of the second deposition step for structure
# 'structure_3d'.
save structure=structure_3d
```

Note:

A 2D structure can be obtained as a cut of a 3D structure using the `extract` command with `type=slice` (see [extract on page 437](#)).

Limitations When Processing 2D Structures

Table 2 lists commands that are not supported or have some limitations when processing 2D structures.

Table 2 Commands not supported or not fully supported when processing 2D structures

Command	Functionality when processing 2D structures
<code>add_litho_command</code>	Sentaurus Lithography integration only works in three dimensions.
<code>define_boundary_conditions</code>	There is no support for nondefault boundary conditions for indirect flux computation for 2D structures.
<code>define_litho_machine</code>	Sentaurus Lithography integration only works in three dimensions.
<code>define_mask</code>	Masks are only supported to process 3D structures.
<code>etch</code>	Supported except for the <code>mask</code> parameter and except when using a reaction model.
<code>filter_structure</code>	Supported except for <code>type=convert_to_pmc</code> , <code>type=rediscretize_boundary</code> , and <code>type=smooth</code> .
<code>litho</code>	Sentaurus Lithography integration only works in three dimensions.
<code>pattern</code>	Patterning is only supported to process 3D structures.

Coordinate Systems

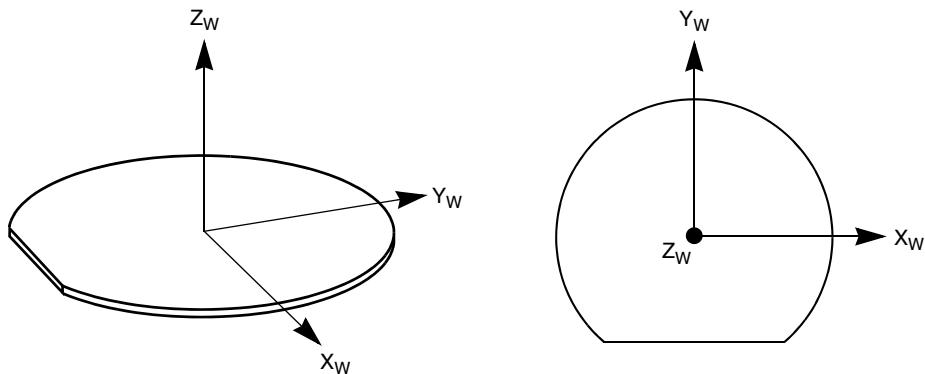
This section describes the wafer coordinate system and the simulation coordinate system.

Wafer Coordinate System

Similar to Sentaurus Process, Sentaurus Topography 3D uses a wafer coordinate system to describe the crystal orientation of the wafer. The wafer coordinate system is a right-handed coordinate system in which the x-axis is parallel to the wafer flat, and the y-axis is perpendicular to the wafer flat. The z-axis is perpendicular to the wafer surface (see [Figure 4](#)).

The tilt and rotation of the structure are defined with respect to the wafer coordinate system (see [Structure Tilt on page 37](#)).

Figure 4 Wafer coordinate system



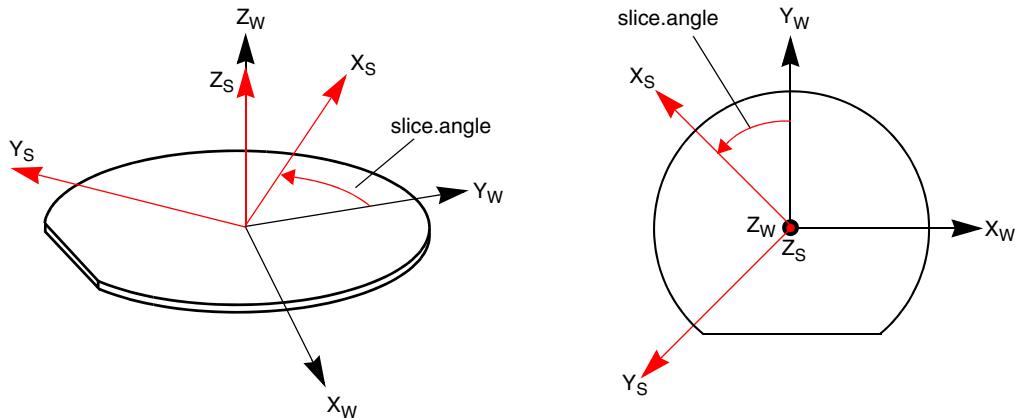
Simulation Coordinate System

In contrast to the simulation coordinate system of Sentaurus Process, in the simulation coordinate system of Sentaurus Topography 3D, the x-axis and y-axis lie in the wafer plane, and the z-axis is perpendicular to the wafer surface. The x-axis of the simulation coordinate system is rotated with respect to the y-axis of the wafer coordinate system by the slice angle (see [Figure 5](#)).

Chapter 2: Simulation Details

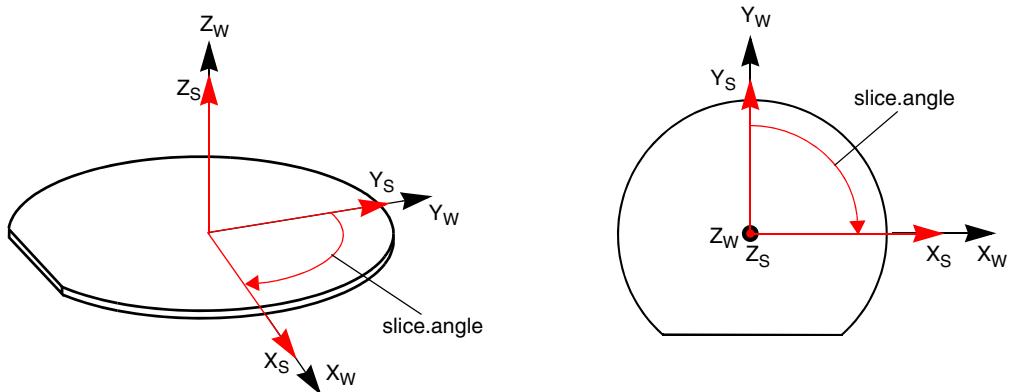
Coordinate Systems

Figure 5 *Simulation coordinate system with slice.angle = 45°*



As in Sentaurus Process, the default value of the slice angle is -90° (see [Figure 6](#)).

Figure 6 *Simulation coordinate system when using default value of slice.angle (-90°)*



The simulation coordinate system is used to specify the coordinates of the simulated structure and all input and output coordinates, except for the crystal orientation.

2D Coordinate System

The simulation coordinate system (x/y) used for 2D structures is oriented in such a way that the positive y-axis points upwards in a device. Therefore, the y-coordinate of the simulation coordinate system used for 2D structures corresponds to the z-coordinate of the simulation coordinate system used for 3D structures.

Structure Tilt

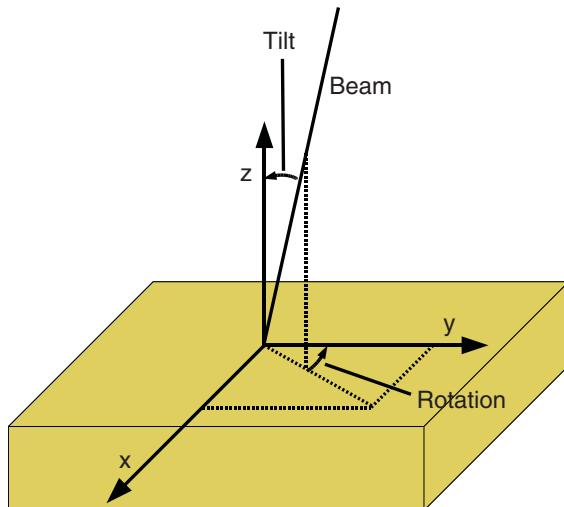
When a machine is defined using either the `define_deposit_machine` command or the `define_etch_machine` command, you can specify the tilt of the structure by setting the parameters `tilt` and `rotation`, which represent the tilt and rotation (or twist) angles as shown in [Figure 7](#).

The tilt is the angle between the beam and the z-axis of the wafer coordinate system. The rotation is defined as the angle between the following two planes:

1. The plane that contains the beam and the z-axis of the wafer coordinate system.
2. The yz plane of the wafer coordinate system.

The tilt angle is positive when measured from the beam axis to the z-axis; while the rotation angle is positive when measured from plane 1 to plane 2 as shown in [Figure 7](#).

Figure 7 Definition of tilt and rotation angles



Material Names and Aliases

By default, when using material names defined in the `datexcodes.txt` file, these names are translated to the canonical name for the specified material. For example, when specifying PolySilicon, it is translated to the canonical name PolySi. Similarly, the material name Resist is translated to Photoresist.

Although using DATEX material aliases can be helpful in large simulation setups where different material names are used, which traditionally refer to the same material, it also can

Chapter 2: Simulation Details

Boundary Conditions

make some simulation setups more difficult to understand. Therefore, the use of DATEX material aliases can be deactivated with the command-line option `--use_datex false`.

Boundary Conditions

Similar to other types of simulation, topography simulations usually handle only a small part of a much larger structure. Typical reasons for this are limited computational resources or a limited area of interest. When limiting the simulation domain to a small part of a larger structure, it is necessary to use boundary conditions to take into account how the parts outside the simulation domain influence the simulation domain.

In general, for some quantities, it is sufficient if the boundary conditions model the immediate vicinity of the simulation domain and, in general, highly accurate results can be obtained. For nonlocal effects, much larger parts outside the simulation domain have a significant influence. This makes the definition of boundary conditions that lead to highly accurate results much more difficult.

For a plasma etching or deposition process, the ion or neutral flux arriving at a point on the surface of the wafer is such a nonlocal effect and can depend on parts of the surface that do not belong to the actual area of interest. Depending on the particular structure, it might still be possible to define boundary conditions that allow you to restrict the simulation domain to the area of interest and to achieve highly accurate results. Unfortunately, this is not always possible.

In cases where limiting the simulation domain to the area of interest and achieving high accuracy is not possible, it is necessary to choose the simulation domain larger than the area of interest.

When increasing the simulation domain, you need to find a trade-off between the improved accuracy in the area of interest and the increase in the required computational resources.

When simulating etching or deposition processes, different boundary conditions are available in Sentaurus Topography 3D: `reflective`, `none`, and `periodic`. The default for the boundary conditions at the sidewalls of the simulation domain is `reflective`, which implements reflective boundary conditions.

The `define_boundary_conditions` command specifies the boundary conditions to use when processing a structure (see [define_boundary_conditions on page 207](#)). However, you can specify periodic boundary conditions only when processing structures using PMC-based models. Periodic boundary conditions are activated automatically whenever you use a model that utilizes the RFM function `pad_pressure()` (see [Data Available for Rate Calculation on page 574](#)) or when processing tilted structures using PMC-based models, as clarified in the following.

For tilted structures, at sidewalls that are not parallel to the tilt vector, boundary conditions of type `reflective` cannot be used. Therefore, another type of boundary condition must be

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Boundary Conditions

applied at those sidewalls, independently of the boundary conditions that were specified for the sidewalls using the `define_boundary_conditions` command. When using level set-based models, the boundary condition type `none` is always enforced on such sidewalls; whereas, periodic boundary conditions are applied when using PMC-based models.

Boundary Conditions: reflective

In general, with reflective boundary conditions, it is assumed that the sidewalls of the simulation domain are symmetry planes. When checking the visibility of the plasma source or other parts of the surface in a specific direction, a ray is started in this direction and the first intersection with the plasma source, the surface, or the sidewalls of the simulation domain is calculated. If the plasma source or the surface is hit, the process stops. If a sidewall of the simulation domain is hit, the ray is reflected and the next intersection is calculated.

In theory, this corresponds to an infinitely extended surface and gives the correct result if the sidewalls of the simulation domain are symmetry planes. In practice, it is necessary to limit the number of reflections and, thereby, to reduce the size of the extended surface that is taken into account. As long as this limit is high enough, it will not have a significant influence on the result.

When calculating the indirect flux using the radiosity method, it is necessary to solve an equation system. The elements of the system matrix depend on the material properties of the surface and on the geometry of the surface.

Radiosity Method

The geometric interaction between a pair of surface elements is described by the form factor. The form factor must be calculated for all pairs of elements of the original surface. However, it is also necessary to calculate the form factors between elements of the original surface and elements that are part of the extended surface, which was created by reflecting the original surface at the sidewall of the simulation domain where the boundary condition type is `reflective`. At corners where both adjacent sidewalls have the boundary type `reflective`, the surface must be extended for the corner area. This is performed by reflecting the original surface at each of these sidewalls, and the form factors between these elements and the elements of the original surface are calculated.

The complexity of calculating the form factors between elements of the original surface and elements of the extended surface increases rapidly with the number of reflections that were necessary to create the surface element. Therefore, the extended surface is limited to the direct neighbors at the sidewalls and at the corners of the simulation domain.

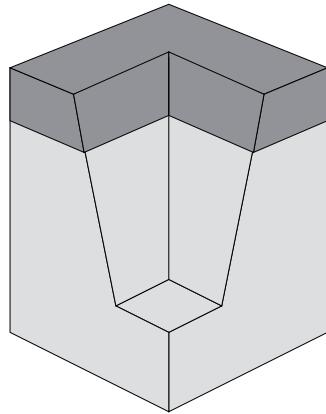
Therefore, the accuracy of the indirect flux calculated using the radiosity method strongly depends on the characteristic of the surface within the simulation domain. For example, if the surface inside the simulation domain represents a quarter or a half of a hole (see

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Boundary Conditions

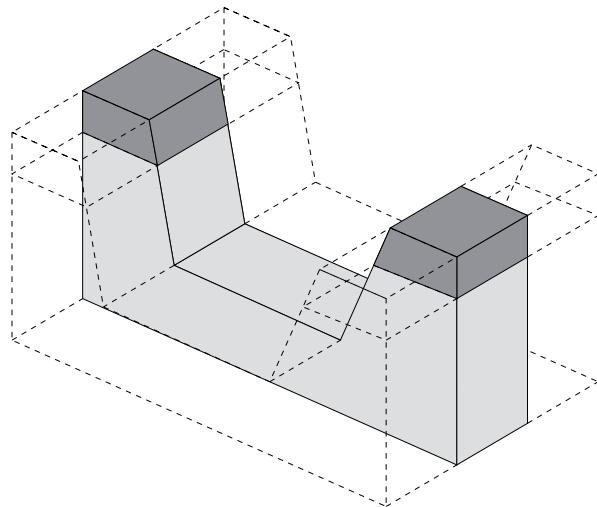
[Figure 8](#)), the interaction of a surface element inside the simulation domain will be limited to other surface elements inside the simulation domain and to elements of the extended surface that were created by one reflection. In this case, the reflective boundary conditions describe the real situation very well, and the result will be highly accurate.

Figure 8 Quarter of a hole



If the surface inside the simulation domain represents the narrow cross section of a trench (see [Figure 9](#)), surface elements much further away than one reflection can have a significant influence. In this case, the result can contain large errors, and it is recommended to use the 2D mode for this kind of structure.

Figure 9 Trench with extended surface at the front and rear sidewalls; the surface is extended at the left and right sidewalls and at the corners but, for this structure, these extensions have no influence on the result and, therefore, are not shown



Boundary Conditions: none

When using the boundary condition type `none`, there is no reflection and no calculation of the next intersection when the ray hits the sidewall of the simulation domain. Boundary conditions of type `none` are not supported when using the PMC method.

When calculating the direct flux, the rays are started from the surface. If a ray hits a sidewall for which the boundary condition type is `none`, the process stops and the plasma source is considered to be visible.

When calculating the indirect flux, the original surface is not extended at sidewalls with the boundary condition type `none`. Therefore, there is no contribution to the indirect flux from elements that would be located in this area.

Boundary Conditions: periodic

When using periodic boundary conditions, the processed structure is supposed to repeat infinitely many times along the direction where periodic boundary conditions are applied.

Periodic boundary conditions can be applied only to a pair of parallel sidewalls and not to a single sidewall. You can specify boundary conditions of type `periodic` only when simulating structures with the PMC method. Periodic boundary conditions are always used for simulating tilted structures with the PMC method as well as for RFM models that utilize the RFM function `pad_pressure()`.

Parallelization

Sentaurus Topography 3D can use multiple CPU cores or CPUs to accelerate simulations on shared-memory computers and on distributed processing (DP) systems. Distributed computation is implemented using the message passing interface (MPI) [2].

Shared-memory parallelization (SMP) on the nodes of a DP system is also supported.

Basic Shared-Memory Parallelization

To activate multithreaded computation, use the command:

```
let parallel=true
```

The number of threads is determined automatically, depending on the hardware resources, the optimum number of threads for the algorithm used, and the number of parallel licenses available. This is the recommended SMP mode.

Advanced Shared-Memory Parallelization Options

Advanced users can set a specific number of threads per process using the command:

```
let num_threads=<n>
```

where `<n>` is an integer greater than zero. This forces Sentaurus Topography 3D to use the number of threads specified for each process. The engine tries to check out the necessary number of parallel licenses.

You can also set the number of threads per process using the `--threads` command-line option (see [From the Command Line on page 17](#)). When doing so, the number of threads specified using the `parallel` and `num_threads` parameters of the `let` command are ignored.

You can use the `--max_threads` command-line option to set the maximum number of threads per process.

If insufficient licenses are available, the behavior of the simulator is controlled by the `parallel_license` parameter of the `let` command (see [let on page 501](#)).

Parallelization on Distributed Processing Systems Using MPI

Sentaurus Topography 3D supports parallelization on distributed processing (DP) systems using the message passing interface (MPI) [2].

To activate parallelization on DP systems, specify a number of processes greater than 1 with the `--processes` command-line option when starting Sentaurus Topography 3D (see [From the Command Line on page 17](#)).

You can specify the hosts where to start the processes using the `--mpi-file` command-line option (see [From the Command Line on page 17](#)).

For details, see *TCAD Parallelization Environment Setup User Guide*, Parallelization Using the Message Passing Interface, and Running TCAD Sentaurus Tools on a Cluster.

In Sentaurus Topography 3D, only PMC simulations and the flux integration using the Monte Carlo method for level set-based models (see [Modeling Fluxes and Related Physical Effects on page 44](#)) can be parallelized on DP systems.

In particular, you can distribute the execution of the following commands over different processes, which can run either on the same host or on the hosts of a cluster:

- `deposit` command, when issued with `engine=monte_carlo`
- `etch` command, when issued with `engine=monte_carlo`
- `etch` command, when issued with `method=pmc`

Chapter 2: Simulation Details

References

Each process executing these commands can use multiple CPU cores or CPUs of the host where it is running, that is, Sentaurus Topography 3D supports SMP on each process of a DP system. See [Basic Shared-Memory Parallelization on page 41](#) and [Advanced Shared-Memory Parallelization Options on page 42](#).

Note:

For best performance, the total number of threads requested on each node must not exceed the number of CPU cores available on the node.

When running on a cluster, the speedup is limited by the performance of the slowest node and by the speed and bandwidth of the network connections between machines. Therefore, for best performance, use cluster machines with uniform performance and with fast interconnections between them.

References

- [1] R. Courant, K. Friedrichs, and H. Lewy, “On the Partial Difference Equations of Mathematical Physics,” *IBM Journal*, vol. 11, no. 2, pp. 215–234, 1967.
- [2] For information about the MPI Forum, go to <https://www mpi-forum.org>.

3

Model Descriptions

This chapter describes the fundamental theory and assumptions of the physical models used in Sentaurus Topography 3D. In particular, level set-based models, the spin-on-glass deposition model, and the reaction models are addressed.

Level Set-Based Models

This section discusses level set-based models.

Modeling Fluxes and Related Physical Effects

[Figure 10](#) shows an overview of the physical processes relevant to the process models implemented in Sentaurus Topography 3D based on the level-set method.

The source of reactants (in most cases, a plasma) is considered to consist of two kinds of particle: neutrals and ions. Neutrals and ions are assumed to be independent and do not interact with each other. However, they can interact with the surface in various ways, as described in the following.

Moreover, for all plasma processes, the pressure in the reaction chamber is assumed to be very low. Therefore, the mean free path length of ions and neutrals is much larger than the feature size.

Fluxes in Sentaurus Topography 3D are normalized such that a flux integrated on an unshadowed flat surface is equal to one. There are two different kinds of flux:

- Fluxes with an angular distribution that is typically isotropic

These fluxes are suitable for modeling electrically neutral species. Therefore, they will be called neutral fluxes in the following.

It is assumed that neutrals travel in a straight path to the surface without interacting with other particles. On the surface, neutrals react with a certain probability, and deposit or etch material. If they do not react, they are isotropically reemitted from the surface. The reemitted particles can react elsewhere or can be reemitted again.

Chapter 3: Model Descriptions

Level Set-Based Models

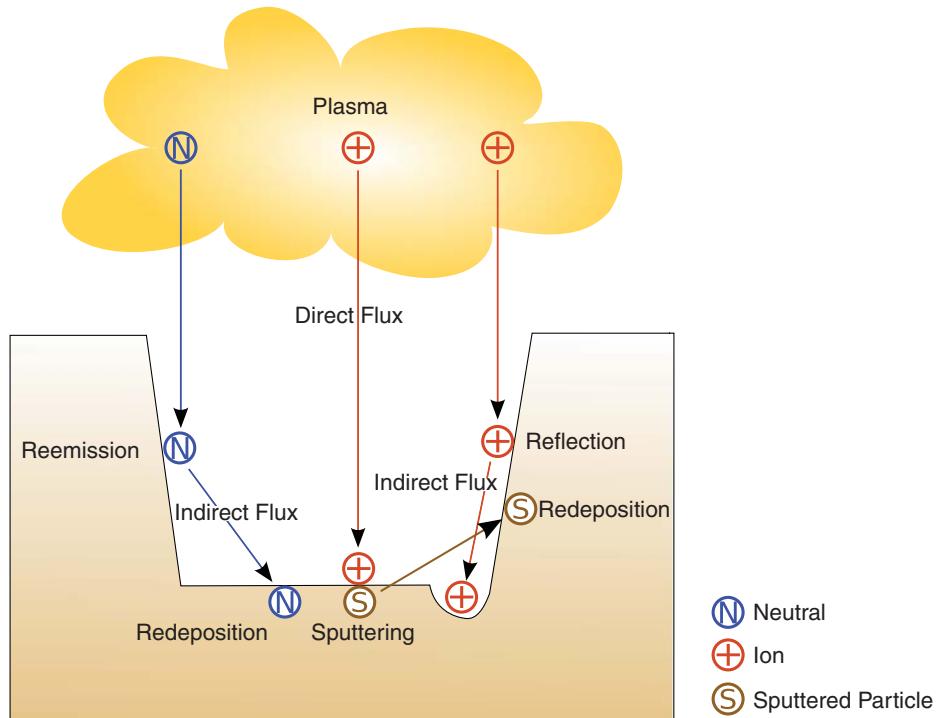
- Fluxes with an anisotropic angular distribution

These fluxes are suitable for modeling charged particles. Therefore, they will be called ion fluxes in the following.

Ions are assumed to travel in a straight path to the surface. Depending on the impinging angle on the surface, ions can then react, or be reflected, or sputter away surface material.

In the case of sputtering or reaction, it is assumed that the ion is consumed. The sputtered particles generate an indirect flux, which can be redeposited elsewhere on the surface. Depending on the material that is being sputtered, the sputtered particles can have an angular distribution with the symmetry axis either normal to the surface or in the direction of the reflected impacting ion.

Figure 10 Physical effects available in Sentaurus Topography 3D for modeling plasma processes



Ion fluxes can have arbitrarily shaped angular distributions. Accordingly, to use a model involving ion fluxes, the angular distributions of each ion flux must be specified (see [define_iad on page 274](#)). Ion angular distributions are properties only of the particles and the processing conditions, and they do not depend on the particular structure under process.

Chapter 3: Model Descriptions

Level Set-Based Models

On the other hand, the distributions of neutral fluxes are supposed to be uniform by default. Therefore, no distribution needs to be defined explicitly for neutral fluxes. However, if needed, this is possible (see [define_nad on page 290](#)).

Neutral and ion fluxes are also different in terms of the physical effects they support.

For neutral fluxes, only reemission is taken into account, which means that a part of the neutrals reaching the surface reacts and sticks to the surface; whereas, the remainder is reemitted isotropically. This effect is characterized by the sticking coefficient according to [Equation 2 on page 48](#).

For each neutral flux, a sticking coefficient must be provided to allow the computation of the reemitted flux. The total number of neutral particles reaching a surface point per unit area and time, taking into account both those directly arriving from the plasma and those reemitted from the surface, is referred to as the *total flux*.

For ion fluxes, it is possible to take into account three physical effects: reflection, sputtering, and deposition of the sputtered material. If reflection is activated, ions can be reflected specularly at the surface of the structure. The reflection probability depends on both the incident angle of the particles and the surface material. As previously mentioned, reflection probabilities are a property not only of the ion flux being reflected, but also of the target material.

Accordingly, to use a model involving reflection, the reflection probability of each ion flux must be known for each material involved in the simulation. The number of particles per unit area and time reaching a surface point after being reflected by all the other surface points is referred to as the *reflected flux*. For built-in models, only the first reflection of ions by the surface is taken into account in the definition of the reflected flux.

If sputtering is taken into account, the number of particles removed from the surface per unit area and time by ions, referred to as the *sputtered flux*, is computed by Sentaurus Topography 3D. The yield function, which gives the number of sputtered atoms per incoming ion as a function of the ion incident angle, is used to specify the process, and it depends on both the properties of the incoming ions and the target material. For this reason, the yield function of each ion flux included in the model must be provided by users for all the materials involved in the structure under process.

Finally, to model reemission of sputtered material, the sticking coefficient, the angular distribution of the sputtered material, and the type of the sputter emission must be provided. For the sputter type `diffuse`, the symmetry axis of the angular distribution of the sputtered material is given by the surface normal. For the sputter type `reflective`, the symmetry axis is defined by the direction of the specular reflection of the incoming ion.

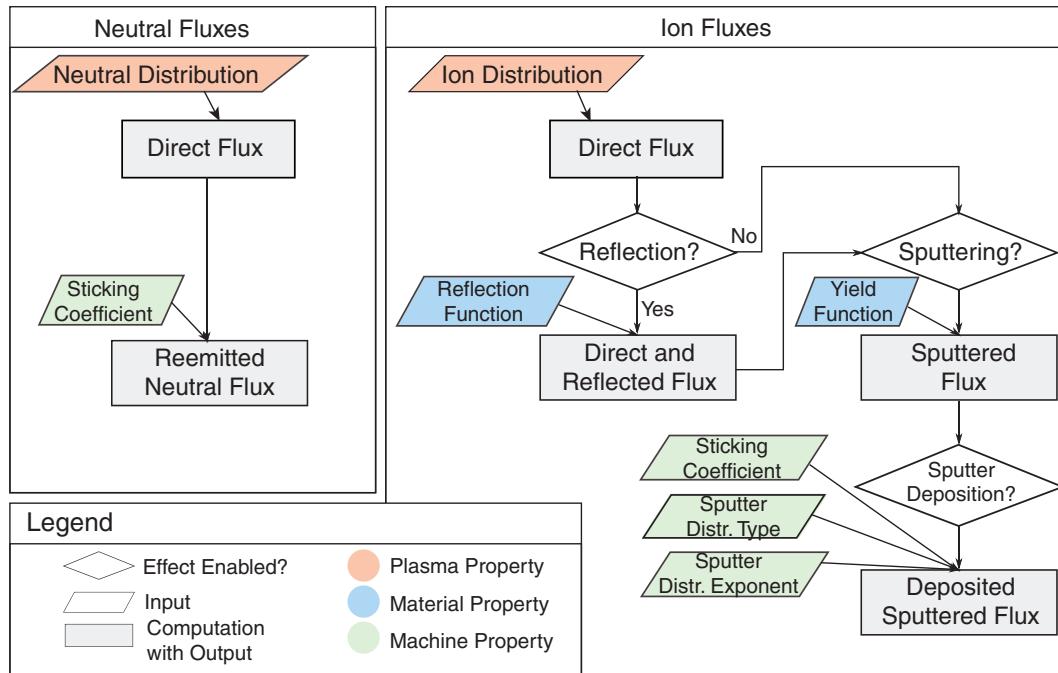
Therefore, the computation of direct and indirect fluxes might require scalar values (such as the sticking coefficient and the sputter type) as well as some functions, for example, ion angular distribution, yield, and reflection functions. Angular distributions are assumed to be only plasma dependent; whereas, yield and reflection functions are specific to both the particles and the target material.

Chapter 3: Model Descriptions

Level Set-Based Models

Figure 11 summarizes the indirect fluxes available in Sentaurus Topography 3D and the information you must provide to compute each of them.

Figure 11 Direct and indirect fluxes and their relationships with physical effects



When a physical effect is activated for a flux, Sentaurus Topography 3D computes the corresponding indirect flux. However, if an indirect flux does not appear in the rate formula, it will have no effect on the evolution of the surface, even if it is computed by Sentaurus Topography 3D. In other words, the definition and the configuration of a flux specify which direct and indirect fluxes are computed at each time step, but the way they are used is defined only by the rate formula. This is important for user-defined models using the rate formula module (RFM) because, for these kinds of model, users are responsible for adding the appropriate fluxes, activating the required physical effects, and defining the rate formula (see [Chapter 8 on page 564](#)).

For built-in models, neutral particles are lumped and modeled as belonging to one flux. The same assumption is made for ion particles in the built-in models. For RFM models, an arbitrary number of ion and neutral fluxes can be used. Each of them can have different properties. [Neutrals on page 48](#) and [Ions on page 50](#) discuss the physical effects in more detail.

Deposition or etching rates for built-in models are obtained by multiplying the normalized flux with the deposition or etching rate measured on an unshadowed flat surface.

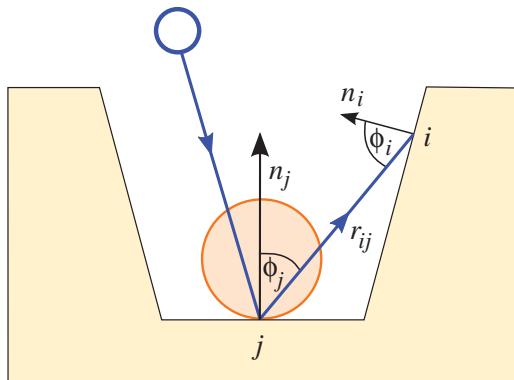
Note:

Level set-based models do not support energy-dependent fluxes.

Neutrals

Usually, a neutral flux is characterized by an isotropic source distribution that is modeled as $\cos\theta$. Neutral particles emitted from the source and arriving at a surface point j can directly react on the point j or can be reemitted several times from the surface and react at a surface point i (see [Figure 12](#)).

Figure 12 Reemission of neutrals



The sticking coefficient is defined as the reaction probability with the surface:

$$\sigma_j = \frac{\Gamma_{\text{reaction},j}}{\Gamma_{\text{neutral},j}} = 1 - \frac{\Gamma_{\text{re-emitted},j}}{\Gamma_{\text{neutral},j}} \quad (1)$$

where:

- $\Gamma_{\text{neutral},j}$ is the total incoming neutral flux at surface element j .
- $\Gamma_{\text{reaction},j}$ is the fraction of the incoming flux that reacts.
- $\Gamma_{\text{re-emitted},j}$ is the fraction of the incoming flux that is reemitted.

The sticking coefficient σ_j is not a constant on the whole surface. It depends on the material at the surface point j but not on the neutral species, and it varies between 0 and 1.

The total neutral incoming flux on a surface point i can be written as the summation of the direct neutral flux plus all the contributions due to reemissions of the surrounding points j [1]:

$$\Gamma_{\text{neutral},i} = \Gamma_{\text{direct},i} + \sum_{j \neq i} (1 - \sigma_j) g_{ij} \Gamma_{\text{neutral},j} \quad (2)$$

where:

- $\Gamma_{\text{direct},i}$ is the direct flux arriving from the source at the point i .
- g_{ij} is the *form factor* that accounts for how much of the reemitted flux from the point j arrives at the point i .

Chapter 3: Model Descriptions

Level Set-Based Models

The form factor depends on the surface geometry and the reemission angular distribution. Assuming that neutrals are reemitted with an isotropic angular distribution [1] (see [Figure 12 on page 48](#)):

$$g_{ij} = \int_{A_j} \frac{\cos\phi_i \cos\phi_j}{\pi r_{ij}^2} V_{ij} dA_j \quad (3)$$

where:

- dA_j is the area of the infinitesimal emitter.
- ϕ_i is the angle between the incoming particle direction and the surface normal.
- ϕ_j is the angle between the emitted particle direction and the normal of the surface of the emitter.
- r_{ij} is the distance between the two surface elements i and j .
- V_{ij} is the mutual visibility matrix, defined as:

$$V_{ij} = \begin{cases} 0 & i \text{ and } j \text{ are not mutually visible} \\ 1 & i \text{ and } j \text{ are mutually visible} \end{cases} \quad (4)$$

[Equation 2](#) is one row of a system of equations that must be solved to find the unknown neutral fluxes $\Gamma_{\text{neutral},i}$ at each surface point.

Analytic Angular Distribution

A good approximation to measured neutral angular distributions (NADs) can be obtained by defining the NAD analytically as:

$$f(\theta) = A \cos^m(\theta) \quad (5)$$

where:

- θ is the angle between the vertical and the incoming neutral direction.
- m is a user-defined parameter (exponent) that describes the anisotropy of the distribution.
- A is a constant that is determined by normalizing the integrated neutral flux on a flat unshadowed surface.

The default NAD is obtained from [Equation 5](#) with $m = 1$.

The flux normalization implies that the normalized flux is dimensionless. Consequently, the total etching or deposition rate can be obtained by multiplying the integrated and normalized flux on a surface element by the etching or deposition rate of a flat unshadowed surface.

Chapter 3: Model Descriptions

Level Set-Based Models

User-Defined Neutral Angular Distribution

The flux models of Sentaurus Topography 3D allow the definition of user-defined NADs, which can be obtained by measurement or from plasma simulations. Arbitrary NADs can be defined or loaded using the `define_nad` command (see [define_nad on page 290](#)). NADs are defined in a tabular format, and linear interpolation is used between data points.

User-defined NADs will be normalized internally when used in flux models.

Ions

The ion flux is characterized by a directional angular source distribution. The source distribution is either modeled as $\cos^m\theta$, where the exponent m controls the flux anisotropy, or specified as an arbitrary ion angular distribution (IAD), using the command `define_iad` (see [define_iad on page 274](#)) and the parameter `iad` in the respective etching or deposition models.

Ions can react on the surface and can etch or deposit. They also can sputter some material from the substrate or be reflected by vertical walls producing the microtrenching phenomenon at the bottom of a trench.

Analytic Ion Angular Distribution

A good approximation to measured IADs can be obtained by defining the IAD analytically according to [Equation 5](#).

As for neutrals, the flux normalization implies that the normalized flux is dimensionless. Consequently, the total etching or deposition rate can be obtained by multiplying the integrated and normalized flux on a surface element by the etching or deposition rate of a flat unshadowed surface.

User-Defined Ion Angular Distribution

The flux models of Sentaurus Topography 3D allow the definition of user-defined IADs, which can have been obtained by measurement or from plasma simulations. Arbitrary IADs can be defined or loaded using the `define_iad` command (see [define_iad on page 274](#)). The IADs are defined in a tabular format, and linear interpolation is used between data points.

User-defined IADs will be normalized internally when used in flux models.

Sputtering

High-energy ions can sputter some substrate material. The sputter etch rate depends greatly on the impact angle θ_{im} of the ions (the angle between the normal of the surface element and the incoming ion direction; see [Figure 13 on page 51](#)).

Chapter 3: Model Descriptions

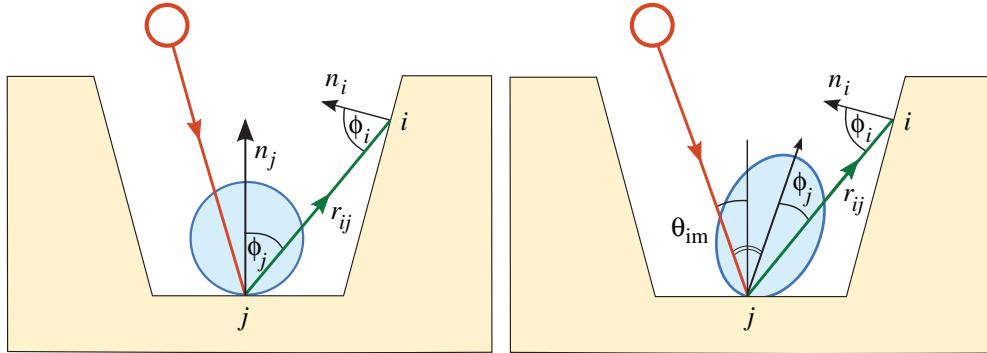
Level Set-Based Models

This dependency is expressed by the yield function:

$$\gamma(\theta_{im}) = s_1 \cos \theta_{im} + s_2 \cos^2 \theta_{im} + s_4 \cos^4 \theta_{im} \quad (6)$$

where s_1 , s_2 , and s_4 are the sputtering coefficients.

Figure 13 Sputtering with the symmetry axis of the angular distribution (left) along the surface normal and (right) along the reflected impacting ion direction



In Sentaurus Topography 3D, the sputtered flux is evaluated under the assumption of a narrow angular distribution (a large coefficient m in the angular distribution) for which it is possible to write:

$$\Gamma_{\text{sputter},j} = \gamma(\theta_{im}) \Gamma_{\text{ion}} \quad (7)$$

where Γ_{ion} is the total direct ion flux, which is normalized. For the sputtered flux Γ_{sputter} to be normalized such that the total sputtered flux from an unshadowed flat surface is unity, it is necessary that $\gamma(0) = 1$. Using this constraint, a relevant condition on the sputtering coefficients is obtained:

$$s_1 + s_2 + s_4 = 1 \quad (8)$$

This means that for the definition of the yield function $\gamma(\theta_{im})$, only two parameters are required, and Sentaurus Topography 3D uses the parameters s_1 and s_2 .

The sputtered material can be redeposited as well. It is assumed that the redeposition process occurs with a probability $\sigma_{\text{redeposit}}$, and no further reemissions are considered, that is, the remaining $1 - \sigma_{\text{redeposit}}$ sputtered material is considered to be volatile. The redeposition flux is:

$$\Gamma_{\text{redeposition},i} = \sigma_{\text{redeposit}} \sum_{j \neq i} v_{ij} \Gamma_{\text{sputter},j} \quad (9)$$

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Level Set-Based Models

where v_{ij} is another form factor that accounts for how much of the sputtered material from the point j arrives at the point i :

$$v_{ij} = \int_{A_j} (m+1) \frac{\cos\phi_i \cos^m \phi_j}{\pi r_{ij}^2} V_{ij} dA_j \quad (10)$$

where ϕ_j now has a general meaning as the angle between the emitted particle direction and the symmetry axis of the angular distribution of the sputtered material (see [Figure 13 on page 51](#)).

The differences between g_{ij} and v_{ij} are:

- g_{ij} is evaluated under the assumptions that the reemission of neutrals can be approximated with an isotropic angular distribution. The symmetry axis of the angular distribution is the surface normal, and the exponent of the cosine distribution is one.
- v_{ij} is evaluated under more general assumptions. Depending on the surface, the angular distribution of the sputtered material can be either:
 - Diffuse – The sputtered particles have no *memory* of the impact direction, and the axis of the distribution is normal to the surface element (see [Figure 13 \(left\)](#)).
 - Reflective – The sputtered particles keep some momentum of the impacting ion, and the axis of the distribution has a preferential direction, which is the reflected incoming ion direction (see [Figure 13 \(right\)](#)).

In both cases (diffuse and reflective), an exponent can be assigned to the angular distribution.

Reflection

Low-energy ions with a large incident angle have a larger probability of being reflected by walls (see [Figure 14](#)). This is an important phenomenon that contributes to microtrenching at the bottom of sidewalls. The probability that an ion is reflected is modeled according to [2]:

$$P_{\text{reflection}}(\theta_{\text{im}}) = \min \left\{ 1, k \left[\frac{1}{2\pi} + \left(\frac{\pi}{4} - \frac{1}{3} \right) \frac{1}{\left(\frac{\pi}{2} - \theta_{\text{im}} \right)^2} + \frac{5}{\pi^3} \left(\frac{\pi}{2} - \theta_{\text{im}} \right) \right] \right\} \quad (11)$$

where k is a constant that depends on the mass and atomic number of the incoming ion and the wall material, and on the ion energy:

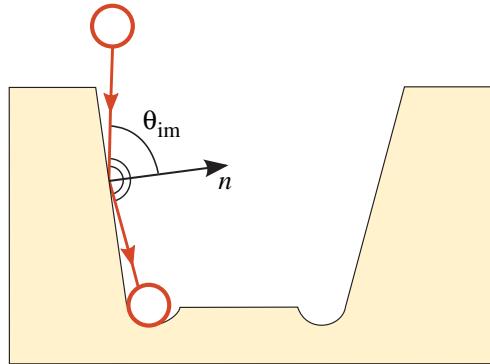
$$k \propto \frac{1}{E_{\text{ion}}^2} \quad (12)$$

The constant k can be set for each material in the structure using the parameter `reflection` in the `add_material` command and the `define_deposit_machine` command (see [add_material on page 177](#) and [define_deposit_machine on page 220](#)).

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Level Set-Based Models

Figure 14 Ion reflection process: ions with a large impact angle can be reflected and react at the bottom of a trench producing microtrenching



Numeric Modeling

The number of incoming (neutral or ion) particles on a surface element is calculated by integrating the various contributions to the total flux. Sentaurus Topography 3D offers two different numeric methods to perform the flux integration: the radiosity method and the Monte Carlo method.

You set the integration method with the parameter `engine` in the `etch` and `deposit` commands. Some models do not support both methods. Furthermore, models that do not perform any flux integration do not need or support these two methods.

Note:

For 2D structures, the only supported flux integration method is the radiosity method.

Table 3 Deposition and etching models: Support for numeric integration methods

Model	Radiosity support	Monte Carlo support
Deposition		
ald	Yes	Yes
crystal	No	No
electrodeposition	No	No
electroplating	No	No
hdp	Yes	Yes
hdp2	Yes	Yes

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Level Set-Based Models

Table 3 Deposition and etching models: Support for numeric integration methods

Model	Radiosity support	Monte Carlo support
lpcvd	Yes	Yes
pecvd	Yes	Yes
pvd	Yes	Yes
simple	No	No
Etching		
crystal	No	No
dry	Yes	Yes
etchdepo	Yes	Yes
etchdepo2	Yes	Yes
hdp	Yes	Yes
hdp2	Yes	Yes
ion_enhanced	Yes	Yes
ionmill	No	No
rie	Yes	Yes
rie2	Yes	Yes
simple	No	No
wet	No	No

Radiosity Method

The radiosity method is a numeric method that solves [Equation 2 on page 48](#) by evaluating the direct flux Γ_{direct} and then by inverting the linear system matrix to find the unknown fluxes at each surface point.

The linear system matrix scales with the square of the number of surface elements and, therefore, it can become prohibitively large for simulations with small level-set grid spacing. In addition, inverting the system matrix does not lend itself well to parallelization and,

Chapter 3: Model Descriptions

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therefore, simulations can use more wallclock time than the Monte Carlo method on multicore machines.

The radiosity method is used by default. It is activated explicitly using `engine=radiosity` in the `etch` and `deposit` commands.

Note:

The following limitations apply:

- The only supported flux integration method for 2D structures is the radiosity method.
- The boundary condition type `reflective` is not supported for the indirect flux calculation for 2D structures.
- The radiosity method does not provide accurate results for machines with a tilt angle greater than approximately 70° for 3D structures.

Monte Carlo Method

In the Monte Carlo method, neutral or ion particles are sent randomly from the top of the simulation domain to the structure. These particles interact with the surface and can be adsorbed or reemitted, and can sputter some material. The particles can be reemitted several times from the surface depending on the sticking coefficient.

The Monte Carlo method uses less memory than the radiosity method because there is no large system matrix to invert. The simulation of individual particles scales well on multiple cores and DP systems. Therefore, the Monte Carlo method shows significant speedup on multicore machines when run in parallel and on DP systems (see [Parallelization on page 41](#)).

You activate the Monte Carlo method using `engine=monte_carlo` in the `etch` and `deposit` commands.

Note:

When using the Monte Carlo method, be careful with the following:

- Due to its stochastic nature, the Monte Carlo method introduces some numeric noise. Therefore, the results of the radiosity method and Monte Carlo method do not always match exactly. The parameter `integration_samples` can be used to increase the number of samples. This increases simulation accuracy at a higher computational cost.
- There is no Monte Carlo implementation for 2D structures. Only the radiosity method is available to perform flux integration with 2D structures.
- The Monte Carlo method can be activated only for models that perform flux integration. See [Table 3 on page 53](#) for a list of supported models.

Orientation-Dependent Models

Sentaurus Topography 3D supports two methods for orientation-dependent etching or deposition modeling when using the level-set method: the built-in `crystal` models and the function `directional_value()` in the rate formula module (RFM) (see [Chapter 8 on page 564](#)).

The RFM function `directional_value()` is used to introduce an orientation dependency into the rate formula of an RFM model. This function has three arguments that are the values of an arbitrary quantity for the directions $<100>$, $<110>$, and $<111>$, respectively. Depending on the direction of the normal of a surface element, an appropriately interpolated value of this quantity is returned and can be used in the rate calculation (see [Data Available for Rate Calculation on page 574](#)).

For each region of a structure, the crystal orientation can be defined. When creating a new region with the `define_structure`, `deposit`, or `etch` command, the crystal orientation can be defined with the parameters `flat_orientation` and `vertical_orientation` (see [define_structure on page 360](#), [deposit on page 375](#), and [etch on page 399](#)).

For structures that were loaded from a TDR file and do not yet contain crystal orientations, or to change the orientation of a region, the `set_orientation` command can be used (see [set_orientation on page 547](#)).

Crystal orientations are always specified with respect to the wafer coordinate system (see [Wafer Coordinate System on page 35](#)).

Setting Crystallographic Orientations

When using a model with orientation-dependent rates, the crystallographic orientations must be defined with respect to the wafer coordinate system.

The slice angle, which defines how the simulated structure is oriented with respect to the wafer coordinate system, can be set only with the `define_structure` command (see [Simulation Coordinate System on page 35](#)). For a newly created structure, the slice angle is defined with the parameter `slice_angle`. If a structure is loaded from a TDR file, the slice angle is read from that file, but the value of the slice angle can be overwritten with the parameter `slice_angle` of the `define_structure` command.

The flat orientation and the vertical orientation of a region can be set with the following commands:

- `define_structure` (only if it is not used to load a structure from a TDR file)
This command sets the crystallographic orientation of a newly created structure (see [define_structure on page 360](#)).
- `deposit` (see [deposit on page 375](#))

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- `etch` (only when using a model for simultaneous etching and deposition; see [etch on page 399](#))
- `set_orientation` (see [set_orientation on page 547](#))

This command sets the crystallographic orientation of any region of a structure.

Note:

The parameters `flat_orientation` and `vertical_orientation` of the `define_structure` command are optional (without a default value). Unless specified, no crystallographic orientation will be set for a newly created region.

The parameters `flat_orientation` and `vertical_orientation` of the `etch` and `deposit` commands are mandatory if the crystallographic orientation is required by the model, namely, for the `crystal` deposition model and RFM models that use the `directional_value()` function in the rate formula. Otherwise, these two parameters are optional (without a default value).

Continuously Rotating and Tilted Structure Modeling

You can model etching, deposition, and simultaneous etching and deposition processes for tilted structures with a continuously increasing value of their rotation angle (see [Structure Tilt on page 37](#)).

This feature is available only for rate formula module (RFM) models and reaction models, and is activated by setting `rotation=continuous` in the `define_deposit_machine` command or the `define_etch_machine` command (see [define_deposit_machine on page 220](#) and [define_etch_machine on page 242](#)).

The simulation of processes involving continuously rotating structures is based on the assumption that the structure rotation period is much smaller than the process time.

To simulate such processes, Sentaurus Topography 3D internally recasts the actual problem into an equivalent one, where the structure of interest is not tilted and does not rotate, and the species of the model (see [add_ion_flux on page 174](#), [add_neutral_flux on page 181](#), and [add_source_species on page 203](#)) have angular distributions different from those of the original problem. Each species of the equivalent problem has the same effect on the not tilted and nonrotating structure as the original species has on the tilted and continuously rotating structure, within a margin of error that depends only on the original angular distribution and on the tilt angle. In the following, such a discrepancy is referred to as the *equivalence error* for a species.

The equivalence error of each species is measured by a number in the range [0, 0.5]. You can set the maximum-tolerated equivalence error for all distributions of a model (parameter `maximum_error` of the `define_deposit_machine` or `define_etch_machine` command). The actual equivalence error of each species of the model is written to the log file, when the machine is used with the `deposit` or `etch` command. If the actual equivalence error for any

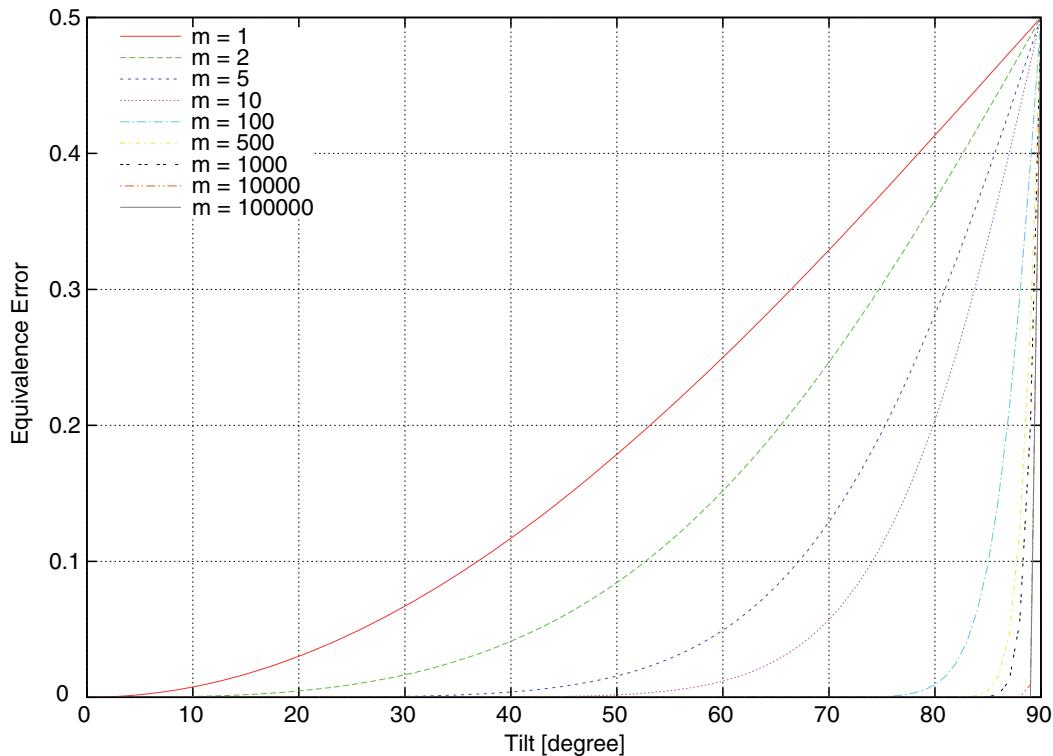
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species of the model is greater than the one specified with the `maximum_error` parameter, an error will be issued.

[Figure 15](#) shows the values of the equivalence error for species having an analytic angular distribution with different values of the exponent m (see [Equation 5 on page 49](#)) for different tilt angles of the structure.

Figure 15 Equivalence error for species having an analytic angular distribution with different values of the exponent for different tilt angles of the structure



As can be seen from [Figure 15](#), the equivalence error increases as the tilt angle increases; whereas, for a given tilt angle, the equivalence error decreases as the angular distribution becomes more focused around the source axis. The trend can be observed for species with angular distributions other than that of [Equation 5](#).

Modeling Chemical-Mechanical Polishing Processes

When using the level-set method, Sentaurus Topography 3D allows you to model chemical-mechanical polishing (CMP) processes at feature scale, using the RFM function `pad_pressure()` (see [Data Available for Rate Calculation on page 574](#)).

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The RFM function `pad_pressure()` returns the pressure produced by a deformable pad in contact with the simulated structure using a contact mechanics-based model [3].

In the implemented model, the pad is characterized by its Young's modulus and Poisson ratio as well as by a Laplacian distribution of the heights of its asperities. The interaction between the pad asperities and the substrate is modeled according to the laws governing Hertz contacts [3].

The Young's modulus of the pad and its Poisson ratio are set with the parameters `pad_young_modulus` and `pad_poisson_ratio` of the `define_etch_machine` command, respectively. Whereas, the standard deviation of the height distribution of the pad asperities is determined from the value of the parameter `pad_roughness` of the `define_etch_machine` command. The pressure applied to the pad is given by the value of the parameter `applied_pressure` of the `define_etch_machine` command (see [define_etch_machine on page 242](#)).

The pressure distribution over the substrate is computed using an iterative method to solve the nonlinear integral equation of the model.

The maximum number of iterations that the solver can perform as well as the solution accuracy below which the solver stops are set with the parameters `pad_pressure_max_iterations` and `pad_pressure_accuracy` of the `etch` command, respectively (see [etch on page 399](#)).

Flux and Flux-Emulating Models

This section presents an overview of the flux and flux-emulating level set-based models available in Sentaurus Topography 3D. Flux and flux-emulating models require flux computations or approximate flux quantities using purely geometric quantities, respectively. See [Deposition Models on page 63](#) and [Etching Models on page 72](#) for detailed descriptions of each model.

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Flux and Flux-Emulating Deposition Models

Table 4 provides an overview of all the flux and flux-emulating deposition models.

Table 4 Flux and flux-emulating deposition models

Model	Machine parameters	Neutral flux with exponent or NAD	Ion flux with exponent or IAD	Reemission and redeposition	Sputtering and redeposition of sputtered material	Diffusive or reflective sputtering
simple	anisotropy curvature rate	No	No	No	No	No
pvd	(exponent iad) rate	No	Yes	No	No	No
lpcvd	(nad neutral_exponent) rate sticking	Yes	No	Yes	No	No
pecvd	anisotropy (exponent iad) (nad neutral_exponent) rate sticking	Yes	Yes	Yes	No	No
hdp	anisotropy (exponent iad) (nad neutral_exponent) rate redeposition s1, s2 sputter_rate sticking	Yes	Yes	Yes	Yes	No

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Table 4 Flux and flux-emulating deposition models (Continued)

Model	Machine parameters	Neutral flux with exponent or NAD	Ion flux with exponent or IAD	Reemission and redeposition	Sputtering and redeposition of sputtered material	Diffusive or reflective sputtering
hdp2	anisotropy (exponent iad) (nad neutral_exponent) rate redeposition reflection s1, s2 sputter_exponent sputter_rate sputter_type sticking	Yes	Yes	Yes	Yes	Yes

Flux and Flux-Emulating Etching and Simultaneous Etching and Deposition Models

[Table 5](#) and [Table 6](#) provide an overview of all the etching, and simultaneous etching and deposition, flux and flux-emulating models.

Table 5 Flux and flux-emulating etching models

Model	simple	ionmill	rie	rie2	hdp	hdp2	ion_enhanced
Machine parameters			(exponent iad)	(exponent iad) (nad neutral_exponent)	(exponent iad)	(exponent iad) (nad neutral_exponent)	(exponent iad) (nad neutral_exponent)
Material parameters	anisotropy curvature rate	anisotropy rate s1, s2	anisotropy rate	anisotropy rate reflection sticking	anisotropy rate s1, s2	anisotropy rate reflection s1, s2 sputter_rate sticking	anisotropy desorption_rate rate reflection s1, s2 sticking

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Table 5 Flux and flux-emulating etching models (Continued)

Model	simple	ionmill	rie	rie2	hdp	hdp2	ion_enhanced
Isotropic etch rate	Yes	Yes	Yes		Yes		
Neutral flux with exponent or NAD				Yes		Yes	Yes
Uni-directional ion flux	Yes	Yes					
Ion flux with exponent or IAD			Yes	Yes	Yes	Yes	Yes
Sputtering		Yes			Yes	Yes	Yes
Reemission				Yes		Yes	Yes
Ion reflection				Yes		Yes	Yes

Table 6 Flux and flux-emulating simultaneous etching and deposition models

Model	dry	etchdepo	etchdepo2
Machine parameters	deposit_material (nad neutral_exponent) rate sticking	deposit_material (exponent iad) rate sticking	deposit_material (exponent iad) (nad (neutral_etch_exponent neutral_exponent)) rate sticking

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Table 6 Flux and flux-emulating simultaneous etching and deposition models (Continued)

Model	dry	etchdepo	etchdepo2
Material parameters	rate s1, s2	rate reflection s1, s2 sputter_type	anisotropy desorption_rate rate reflection s1, s2 sticking
Isotropic etch rate	No	No	No
Neutral flux with exponent or NAD	Yes	No	Yes
Unidirectional ion flux	No	No	No
Ion flux with exponent or IAD	No	Yes	Yes
Sputtering	Yes	Yes	Yes
Diffusive or reflective sputtering	No	Yes	Yes
Reemission	Yes	No	Yes
Redeposition	No	Yes	No
Ion reflection	No	Yes	Yes

Deposition Models

This section discusses deposition models.

Simple Deposition

Set `model=simple` in the `define_deposit_machine` command to define a simple deposition machine (see [define_deposit_machine on page 220](#)).

The deposition rate is evaluated as the contribution of the following components:

- An isotropic deposition
- A directional deposition

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- A curvature-dependent term

The resulting rate at a surface point (x, y, z) can be written as:

$$R(x, y, z) = \begin{cases} R_0[(1 - A) + H(x, y, z)A\vec{v} \cdot \vec{n}(x, y, z)](1 - k\kappa(x, y, z)) & ** \\ 0 & \text{Otherwise} \end{cases} \quad (13)$$

** If (x, y, z) does not lie on the surface enclosing a void or if `exposed_only=false` in the `deposit` command

where:

- A is the anisotropy factor, parameter `anisotropy`.
- $H(x, y, z)$ is a function that accounts for point shadowing in the vertical direction, defined as:

$$H(x, y, z) = \begin{cases} 0 & \text{vertically shadowed region} \\ 1 & \text{vertically unshadowed region} \end{cases} \quad (14)$$

- k is the curvature factor; parameter `curvature`.
- $\kappa(x, y, z)$ is the surface curvature at the point (x, y, z) .
- $\vec{n}(x, y, z)$ is the unit vector normal to the surface at the point of coordinate (x, y, z) .
- R_0 is the deposition rate on a completely flat surface; parameter `rate`.
- \vec{v} is the unit vector normal to the horizontal plane.

The limiting values of $A = 0$ and $A = 1$ correspond to a pure isotropic and a pure directional deposition model.

The pure isotropic deposition model mimics a chemical vapor deposition (CVD) where reactants, or reactive intermediates, have a very low sticking coefficient, resulting in a uniform concentration of reactants along the surface irrespective of the geometric configuration.

The pure directional deposition model corresponds to a physical vapor deposition (PVD) process where deposition occurs in only one direction. Atoms in the vapor stream that impinge on the surface of the structure are always parallel to the vector \vec{v} . No material deposition occurs in the shadowed regions (see [Equation 13](#) and [Equation 14](#)).

The curvature term has the effect of decreasing the deposition at convex surfaces and increasing the deposition at concave surfaces, smoothing the surface as it evolves.

Physical Vapor Deposition

Set `model=pvd` in the `define_deposit_machine` command to define a physical vapor deposition (PVD) machine (see [define_deposit_machine on page 220](#)).

The PVD model applies to processes where the deposition involves pure physical processes rather than chemical reactions. The particle flux is characterized by a $\cos^m\theta$ angular distribution, where m is set by the parameter `exponent` or a user-defined IAD (the parameter `iad`).

The sticking coefficient is equal to one, that is, each incoming particle deposits on the surface. The deposition rate R_0 on an unshadowed flat surface is set with the parameter `rate`.

The total deposition rate is evaluated as:

$$R = R_0 \Gamma \quad (15)$$

where Γ is the integrated flux on the considered surface point.

Low-Pressure Chemical Vapor Deposition

Set `model=lpcvd` in the `define_deposit_machine` command to define a low-pressure chemical vapor deposition (LPCVD) machine (see [define_deposit_machine on page 220](#)).

In the LPCVD model, the vapor flux of chemical precursors is simulated by neutrals having, by default, an isotropic angular flux distribution. The distribution of the neutral flux can be set either by using the parameter `neutral_exponent` or by specifying a user-defined NAD (the parameter `nad`). The incoming particles can either react on the surface and be deposited, with a probability given by the sticking coefficient (parameter `sticking`), or be reemitted as described in [Neutrals on page 48](#). The reemitted flux is distributed isotropically. The deposition rate R_0 on an unshadowed flat surface is set with the parameter `rate`. The total deposition rate is evaluated as:

$$R = R_0 \Gamma_{\text{neutral}} \quad (16)$$

with Γ_{neutral} evaluated from [Equation 2 on page 48](#).

Plasma-Enhanced Chemical Vapor Deposition

Set `model=pecvd` in the `define_deposit_machine` command to define a plasma-enhanced chemical vapor deposition (PECVD) machine (see [define_deposit_machine on page 220](#)).

The incoming fluxes to the surface are characterized by two components: a thermally driven LPCVD precursor and ion-induced deposition precursors. The parameter `anisotropy` sets the ratio between the anisotropic ion rate and the total deposition rate R_0 (parameter `rate`). The ion flux can be defined to have a $\cos^m\theta$ angular distribution, where m is set by the parameter `exponent`, or can be a user-defined IAD (the parameter `iad`). By default, the neutral flux has an isotropic distribution. It can be defined to have a $\cos^m\theta$ angular

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distribution, where m is set by the parameter `neutral_exponent` or can be a user-defined NAD (the parameter `nad`).

The total deposition rate is evaluated as:

$$R = (1 - A)R_0\Gamma_{\text{neutral}} + AR_0\Gamma_{\text{ion}} \quad (17)$$

High-Density Plasma Deposition

Set `model=hdp` in the `define_deposit_machine` command to define a high-density plasma (HDP) deposition machine (see [define_deposit_machine on page 220](#)).

In the HDP deposition model, two simultaneous mechanisms are competing: the deposition and the etching by physical sputtering due to high-energy ions. The neutral flux can either react and be deposited with a probability given by the sticking coefficient σ_j (see [Equation 1 on page 48](#)), the parameter `sticking`, or be reemitted as described in [Neutrals on page 48](#).

Ions are deposited on the surface and, at the same time, can induce a flux of sputtered particles. The sputtering etch rate is highly dependent on the impact angle, and it is described by a yield function (see [Equation 6 on page 51](#)), in which s_1 and s_2 are set with the parameters `s1` and `s2`, respectively.

It is assumed that the sputtered material has an isotropic angular distribution. The amount of redeposition on the surface $\sigma_{\text{redeposition}}$ is set by the parameter `redeposition`.

The total rate on an unshadowed flat surface is given by:

$$R_{\text{flat}} = R_0 - R_{\text{sputter}} \quad (18)$$

where:

- R_0 is the deposition rate on an unshadowed flat surface, without sputtering; parameter `rate`.
- R_{sputter} is the sputtering rate; parameter `sputter_rate`.

Note:

The model assumes a net deposition, that is, $R_0 > R_{\text{sputter}}$ must hold for flat surfaces.

The total deposited material is the sum of the deposition due to neutrals (direct and indirect flux), plus the deposition due to ions, plus the sputtered material that redeposits, minus the amount of locally sputtered material. Finally, for nonzero anisotropy, the deposition rate is:

$$R = (1 - A)R_0\Gamma_{\text{neutral}} + AR_0\Gamma_{\text{ion}} + R_{\text{sputter}}(\Gamma_{\text{redeposition}} - \Gamma_{\text{sputter}}) \quad (19)$$

where A is the anisotropy coefficient; parameter `anisotropy`.

For anisotropy equal to zero, the deposition rate is:

$$R = R_0\Gamma_{\text{neutral}} \quad (20)$$

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The fluxes Γ_{neutral} , $\Gamma_{\text{redeposition}}$, and Γ_{sputter} are evaluated as described in [Neutrals on page 48](#) and [Ions on page 50](#).

High-Density Plasma 2 Deposition

Set `model=hdp2` in the `define_deposit_machine` command to define a high-density plasma 2 (HDP2) deposition machine (see [define_deposit_machine on page 220](#)).

The HDP2 model extends the HDP model. It takes ion reflection into account and allows you to specify the sputter type and sputter exponent.

For nonzero anisotropy, the deposition rate is:

$$R = (1 - A)R_0 \tilde{\Gamma}_{\text{neutral}} + AR_0 \tilde{\Gamma}_{\text{ion}} + R_{\text{sputter}}(\tilde{\Gamma}_{\text{redeposition}} - \tilde{\Gamma}_{\text{sputter}}) \quad (21)$$

For anisotropy equal to zero, the deposition rate is:

$$R = R_0 \Gamma_{\text{neutral}} \quad (22)$$

[Equation 21](#) has the same structure as [Equation 19](#), but the factors $\tilde{\Gamma}_{\text{ion}}$ and $\tilde{\Gamma}_{\text{redeposition}}$ for the ion flux and the redeposition, respectively, are different.

$\tilde{\Gamma}_{\text{ion}}$ takes ion reflection into account as described in [Reflection on page 52](#). When the parameter `reflection` is set to 0, $\tilde{\Gamma}_{\text{ion}}$ is equal to Γ_{ion} in [Equation 19](#).

$\tilde{\Gamma}_{\text{redeposition}}$ can take diffuse or reflective reemission of the sputtered material into account. By setting `sputter_type=diffuse` and `sputter_exponent=1`, $\tilde{\Gamma}_{\text{redeposition}}$ is equal to $\Gamma_{\text{redeposition}}$ in [Equation 19](#).

As in the HDP model, the HDP2 model considers the process with two competing simultaneous mechanisms: the deposition and the etching by physical sputtering due to high-energy ions. The neutral flux can either react and be deposited with a probability given by the parameter `sticking` or be reemitted. Ions are deposited on the surface and, at the same time, can induce a flux of sputtered particles. The angular dependency of the sputter rate is given by the yield function as defined in [Equation 6](#) by the parameters `s1` and `s2`.

The main difference with respect to the HDP model is that the angular distribution of the sputtered material, diffuse or reflective, can be set by users (see [Ions on page 50](#)). The ion reflection index (see [Reflection on page 52](#)) is set with the parameter `reflection`.

The rate evaluation for the HDP2 model is the same as that described in [Equation 19](#).

Atomic Layer Deposition

Set `model=ald` in the `define_deposit_machine` command to define an atomic layer deposition (ALD) machine (see [define_deposit_machine on page 220](#)).

The ALD model is an empirical model that incorporates self-limited growth behavior with a calibration parameter (`conformality`) to control the conformality of the deposited layer.

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Self-limiting growth is achieved by a rate model that empirically describes the self-limiting saturated growth behavior, which is typical for ALD.

Electrodeposition

Set `model=electrodeposition` in the `define_deposit_machine` command to define an electrodeposition machine (see [define_deposit_machine on page 220](#)).

The model takes into account the following species: plating species, inhibitors, and accelerators. They are assumed to diffuse from the bulk of the plating bath to the surface of the structure under processing, with their concentrations remaining constant at a specified distance above the top of the structure.

Inhibitors and accelerators competitively adsorb on the surface of the structure. Their adsorption kinetics are determined by their local concentration, their adsorption rates, and the local surface curvature. The additives surface interaction model also includes displacement of inhibitors by accelerators and surface saturation effects. The local surface coverage of inhibitors and accelerators, together with the local concentration of the species being plated, determine the deposition rate of the plating species.

You can set up an oscillating overpotential between two values with a given duty cycle to simulate pulse-plating conditions.

The deposition rate R of the plating species at each surface element is determined by the local surface coverage of inhibitors and accelerators, by the local concentration of the species being plated, and by the overpotential, as specified by the following equations [\[4\]](#)[\[5\]](#)[\[6\]](#):

$$R = \frac{\Omega}{zF} \frac{C_{\text{depo}}}{C_{\text{depo}}^{\text{ref}}} J \quad (23)$$

where:

$$J = \omega [DC J_{\text{on}} + (1 - DC)J_{\text{off}}] \quad (24)$$

$$J_{\text{on}} = J_0(1 - \vartheta_{\text{accel}} - \vartheta_{\text{inhib}})g(\alpha, \eta_{\text{on}}) + J_0^{\text{accel}}\vartheta_{\text{accel}}g(\alpha_{\text{accel}}, \eta_{\text{on}}) + J_0^{\text{inhib}}\vartheta_{\text{inhib}}g(\alpha_{\text{inhib}}, \eta_{\text{on}}) \quad (25)$$

$$J_{\text{off}} = J_0(1 - \vartheta_{\text{accel}} - \vartheta_{\text{inhib}})g(\alpha, \eta_{\text{off}}) + J_0^{\text{accel}}\vartheta_{\text{accel}}g(\alpha_{\text{accel}}, \eta_{\text{off}}) + J_0^{\text{inhib}}\vartheta_{\text{inhib}}g(\alpha_{\text{inhib}}, \eta_{\text{off}}) \quad (26)$$

$$g(a, \eta) = \exp\left(-a\frac{z_a F}{RT}\eta\right) - \exp\left((1-a)\frac{z_a F}{RT}\eta\right) \quad (27)$$

and:

- Ω is the molar volume of the plating species (parameter `depo_molar_volume`).
- DC is the duty cycle of the electrode overpotential (parameter `duty_cycle`). When its value is 1, pulse plating is deactivated.

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- z is the number of electrons transferred during the deposition of an ion of the plating species (parameter z).
- $F = 96485.33289 \text{ C/mol}$ is the Faraday constant.
- ω is equal to 1 if the current surface element does not belong to a void and is equal to 0 otherwise.
- C_{depo} is the local concentration of the plating species. Its value is computed by the simulator assuming that the concentration of the plating species remains constant to the value specified by the `depo_bulk_concentration` parameter at the distance from the top of the structure given by the `bulk_distance` parameter. The diffusivity of the plating species can be specified with the `depo_diffusivity` parameter. When `depo_diffusivity` is not specified, the concentration of the plating species is assumed to be equal to its bulk value all over the surface. C_{depo} depends on both the electrode overpotential and its duty cycle.
- $C_{\text{depo}}^{\text{ref}}$ is the reference concentration of the plating species at which the exchange current densities are measured (parameter `depo_reference_concentration`).
- J_0 is the exchange current density for a surface where no additives were adsorbed, when the concentration of the plating species is $C_{\text{depo}}^{\text{ref}}$ (parameter `exchange_current_density` parameter).
- J_0^{accel} is the exchange current density for a surface fully covered by accelerators, when the concentration of the plating species is $C_{\text{depo}}^{\text{ref}}$ (`exchange_current_density_acc` parameter).
- J_0^{inhib} is the exchange current density for a surface fully covered by inhibitors, when the concentration of the plating species is $C_{\text{depo}}^{\text{ref}}$ (`exchange_current_density_inh` parameter).
- ϑ_{accel} and ϑ_{inhib} are the local accelerator and inhibitor surface coverages, respectively. Their values are computed by the simulator and depend on the following quantities (among others):
 - Accelerator adsorption rate (parameter `acc_adsorption_rate`).
 - Inhibitor adsorption rate (parameter `inh_adsorption_rate`).
 - Accelerator saturation surface concentration (parameter `acc_saturation_surface_concentration`).
 - Inhibitor saturation surface concentration (parameter `inh_saturation_surface_concentration`).
 - Inhibitor displacement rate by accelerators (parameter `inh_displacement_rate`).
 - Local concentration of accelerators. This value is computed assuming that the accelerator concentration remains constant to the value specified by the

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`acc_bulk_concentration` parameter at the distance from the top of the structure given by the `bulk_distance` parameter. The diffusivity of accelerators can be specified with the `acc_diffusivity` parameter. When `acc_diffusivity` is not specified, the concentration of accelerators is assumed to be equal to its bulk value all over the surface.

- Local concentration of inhibitors. This value is computed assuming that the inhibitor concentration remains constant to the value specified by the `inh_bulk_concentration` parameter at the distance from the top of the structure given by the `bulk_distance` parameter. The diffusivity of inhibitors can be specified with the `inh_diffusivity` parameter.
- Local surface curvature.
- α , α_{accel} , and α_{inhib} are the transfer coefficients (parameters `alpha`, `alpha_acc`, and `alpha_inh`, respectively).
- z_α is the number of electrons transferred during the rate-determining elementary reaction (parameter `z_alpha`).
- $R = 8.3144598 \text{ J/mol/K}$ is the gas constant.
- T is the absolute temperature of the electroplating cell (parameter `temperature`).
- η_{on} is the electrode overpotential during the `on` time of the pulse period when pulse plating is either activated or deactivated (parameter `overpotential`).
- η_{off} is the electrode overpotential during the `off` time of the pulse period when pulse plating is activated (parameter `overpotential_off`).

Electroplating Deposition

Set `model=electroplating` in the `define_deposit_machine` command to define an electroplating machine (see [define_deposit_machine on page 220](#)).

This model applies to the electrodeposition of copper. The deposition rate is proportional to the ratio of accelerators to inhibitors on the surface. The accelerators are conserved as the surface evolves. For trenches, accelerators in the trench accumulate while the trench closes, leading to an accelerated surface growth speed in the trench, an effect that is commonly referred to as *superfilling*.

It is assumed that, at the beginning of a simulation, there is a starting coverage of accelerators distributed on the exposed surface. The initial distribution of accelerators either can be uniform, which is the default, or can be set to be linearly dependent on the depth of the surface. The parameter `delta` describes the derivative of the accelerator coverage with respect to the vertical direction. This parameter is used to emulate an unevenly distributed initial accelerator coverage, where the coverage in the depths of a trench is lower than on the top surface.

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In each time step, the surface evolves; whereas, the deposition rate R at each surface element is proportional to the ratio of accelerator coverage C_{accel} and inhibitor coverage C_{inhib} at the surface element:

$$R \propto R_0 \frac{C_{\text{accel}}}{C_{\text{inhib}}} \quad (28)$$

where:

- R_0 is the deposition rate (parameter `rate`).
- C_{accel} is the accelerator coverage on the surface. The total number of accelerators is conserved over time.
- C_{inhib} is the inhibitor coverage on the surface. It is assumed that inhibitors are constantly replenished from the electrolyte solution and, therefore, inhibitors are distributed uniformly in space, and the coverage remains constant in time.

Crystallographic Orientation–Dependent Deposition

Set `model=crystal` in the `define_deposit_machine` command to define a crystallographic orientation–dependent deposition machine (see [define_deposit_machine on page 220](#)).

The deposition rate is determined by the orientation of the exposed surface with respect to the lattice of its bulk material, which is assumed to be cubic. More precisely, the deposition rate at any point of the exposed surface is computed as the spherical barycentric interpolation [7], along its normal direction, of the deposition rates along the $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ crystallographic directions (parameters `rate_100`, `rate_110`, and `rate_111` of the `define_deposit_machine` command, respectively).

The crystallographic orientation of the deposited material must be defined with the parameters `flat_orientation` and `vertical_orientation` of the `deposit` command. The model does not require the other regions of the structure to have crystallographic orientations defined. See [Orientation-Dependent Models on page 56](#), [Setting Crystallographic Orientations on page 56](#), and [set_orientation on page 547](#).

Moreover, unlike the other deposition models, this model makes it possible to simulate selective deposition processes, as the list of materials on which deposition will occur can be specified using the `selective_materials` parameter of the `define_deposit_machine` command.

Etching Models

This section discusses etching models.

Simple Etching

Set `model=simple` in the `define_etch_machine` command to define a simple etching machine (see [define_etch_machine on page 242](#)).

The etch rate is evaluated as the contribution of the following different components:

- An isotropic etch
- A directional etch
- A curvature-dependent term

The resulting rate at the surface point (x, y, z) for the material m can be written as:

$$R_m(x, y, z) = \begin{cases} R_{0m}[(1 - A_m) + H(x, y, z)A_m\hat{v} \cdot \hat{n}(x, y, z)](1 + k_m\kappa(x, y, z)) & ** \\ 0 & \text{Otherwise} \end{cases} \quad (29)$$

** If (x, y, z) does not lie on the surface enclosing a void or if `exposed_only=false` in the `etch` command

where:

- A_m is the anisotropy factor of material m (parameter `anisotropy`).
- $H(x, y, z)$ is a function that accounts for shadowing, defined in [Equation 14](#).
- k_m is the curvature factor for material m (parameter `curvature`).
- $\kappa(x, y, z)$ is the surface curvature in the point (x, y, z) .
- $\hat{n}(x, y, z)$ is the unit vector normal to the surface at the point of coordinate (x, y, z) .
- R_{0m} is the etching rate on a completely flat surface for material m (parameter `rate`).
- \hat{v} is the unit vector normal to the horizontal plane.

Plasma-assisted processes from reactive or nonreactive ions impinging upon the surface of the structure usually result in a directional etching. The directional component is evaluated only for unshadowed regions (see [Equation 14](#) and [Equation 29](#)).

The curvature term has the effect of increasing etching at convex surfaces and decreasing etching at concave surfaces, smoothing the surface as it evolves.

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Ion-Milling

Set `model=ionmill` in the `define_etch_machine` command to define an ion-mill etching machine (see [define_etch_machine on page 242](#)).

In this model, etching is due to high-energy (unidirectional) ions impacting the surface. The sputtering etch rate is evaluated using the yield function defined in [Equation 7](#):

$$R_m(x, y, z) = R_{0m}[(1 - A_m) + H(x, y, z)A_m\gamma_m(\theta_{im})] \quad (30)$$

where:

- A_m is the anisotropy factor of material m (parameter `anisotropy`).
- $\gamma_m(\theta_{im})$ is the value of the yield function for the material m and the ion impact angle θ_{im} .
- $H(x, y, z)$ is the function that accounts for the surface point shadowing as defined in [Equation 14](#).
- R_{0m} is the etching rate on a completely flat surface for material m (parameter `rate` in the `add_material` command).

Reactive Ion Etching

Set `model=rie` in the `define_etch_machine` command to define a reactive ion etch (RIE) machine (see [define_etch_machine on page 242](#)).

The etching process has two contributions: an isotropic etch and an anisotropic etch. The isotropic etch emulates the wet (chemical) etch process, while the anisotropic etch emulates the plasma etch process.

The anisotropic etch rate is proportional to the incoming ion flux. The ion flux Γ_{ion} either has an angular distribution $\cos^m\theta$, where m is set by the parameter `exponent`, or is a user-defined IAD (the parameter `iad`).

The etch rate R_{0m} on an unshadowed flat surface for the material m is set with the parameter `rate`.

The total etch rate is the sum of these two etch rates:

$$R_m = (1 - A_m)R_{0m} + A_mR_{0m}\Gamma_{ion} \quad (31)$$

where A is the anisotropy coefficient; parameter `anisotropy`.

Reactive Ion Etching 2

Set `model=rie2` in the `define_etch_machine` command to define a reactive ion etch 2 (RIE2) machine (see [define_etch_machine on page 242](#)).

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The RIE2 model extends the RIE model by improving both the neutral and the ion modeling. The RIE2 model considers the etching process as the result of the following contributions:

- Chemical reactions induced by radicals
- Desorptions from the surface induced by ions

The evaluation of the neutral flux Γ_{neutral} is performed considering the structure shadowing and the multiple reemissions as described in [Neutrals on page 48](#) (see [Equation 2](#)). The sticking coefficient is material dependent and must be set during the material definition with the parameter `sticking`. By default, the neutral flux has an isotropic distribution. It can be defined to have a $\cos^m\theta$ angular distribution, where m is set by the parameter `neutral_exponent` or can be a user-defined NAD (the parameter `nad`).

Ion reflection can be included by setting the parameter `reflection` as described in [Reflection on page 52](#). The ion etch rate is proportional to the incoming ion flux. The ion flux has an angular distribution $\cos^m\theta$, where m is set by the parameter `exponent`, or is a user-defined IAD (the parameter `iad`).

The etch rate R_{0m} on an unshadowed flat surface for the material m is set with the parameter `rate`.

The etch contribution due to neutrals and ions is:

$$R_m = (1 - A_m)R_{0m}\Gamma_{\text{neutral}} + A_mR_{0m}\Gamma_{\text{ion}} \quad (32)$$

where A_m is the anisotropy coefficient for material m (parameter `anisotropy`). The flux Γ_{neutral} is evaluated as described in [Neutrals on page 48](#).

High-Density Plasma Etching

Set `model=hdp` in the `define_etch_machine` command to define a high-density plasma (HDP) etching machine (see [define_etch_machine on page 242](#)).

As in the RIE process, the etch rate has two contributions: an isotropic etch and an anisotropic etch. The total etch rate is the sum of these two contributions; the parameter `anisotropy` defines the ratio between the anisotropic etch rate and the total rate. The isotropic etch emulates the wet (chemical) etch process. The anisotropic etch emulates the plasma etch process that, contrary to the RIE model, is due mainly to sputtering. The sputtering yield function is defined as in [Equation 6](#). The anisotropic etch models the plasma etch process where the anisotropic etch rate is proportional to the incoming ion flux. The isotropic part consists of two terms: an isotropic etch term and a term that is proportional to the incoming ion flux. The latter is only active if the surface element is shadowed by another surface element in the vertical direction; whereas, the former is only active if, in the vertical direction, there is no shadowing (see [Equation 14](#)).

The total etch rate is:

$$R_m = (1 - A_m)R_{0m}[H(x, y, z) + (1 - H(x, y, z))\Gamma_{\text{ion}}] + A_mR_{0m}\gamma_m(\theta_{\text{im}})\Gamma_{\text{ion}}H(x, y, z) \quad (33)$$

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where:

- A_m is the anisotropy factor of material m (parameter `anisotropy`).
- R_{0m} is the etching rate on a completely flat surface for the material m (parameter `rate` in the `add_material` command).
- $H(x, y, z)$ is the function that accounts for the surface point shadowing as defined in [Equation 14](#).

The ion flux has an angular distribution $\cos^m\theta$, where m is set by the parameter `exponent`, or is a user-defined IAD (the parameter `iad`).

High-Density Plasma 2 Etching

Set `model=hdp2` in the `define_etch_machine` command to define a high-density plasma 2 (HDP2) etching machine (see [define_etch_machine on page 242](#)).

The HDP2 model extends the HDP model by implementing the features already discussed in [Reactive Ion Etching 2 on page 73](#) for the RIE2 model: neutral flux calculation including reemissions and ion reflections.

The HDP2 model considers etching as the result of the following contributions:

- Chemical reactions induced by radicals
- Desorptions from the surface induced by ions
- Sputtering

The total rate is given by:

$$R_m = (1 - A_m)R_{0m}\Gamma_{\text{neutral}} + A_mR_{0m}\Gamma_{\text{ion}} + A_mR_{\text{sputter}, m}\gamma_m(\theta_{\text{im}})\Gamma_{\text{ion}} \quad (34)$$

where:

- A_m is the anisotropy coefficient for the material m (parameter `anisotropy`).
- $R_{\text{sputter}, m}$ is the sputtering rate for the material m (parameter `sputter_rate`).
- R_0 is the etch rate on a flat unshadowed surface when there is no sputtering (parameter `rate`).
- Γ_{neutral} is the neutral flux that takes shadowing and multiple reemissions into account as described in [Neutrals on page 48](#) (see [Equation 2](#)). The sticking coefficient σ_j is material dependent and must be set during the material definition with the parameter `sticking`.

Ion-Enhanced Etching

Set `model=ion_enhanced` in the `define_etch_machine` command to define an ion-enhanced etching machine (see [define_etch_machine on page 242](#)).

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The ion-enhanced etching model considers etching as the result of the combined effects of neutrals and ions. Neutrals are deposited on the surface (neutral flux Γ_{neutral}). Then, either these neutrals are removed by ions or they dissociate from the surface through thermal desorption. Where the layer of neutrals is removed, chemical etching occurs.

The etching due to ions is modeled as a sputter etching process, where the sputter yield function is defined as in [Equation 6](#).

In this model, the total etch rate is not considered as the linear summation of neutrals and ions etch rates, but:

$$R_m = \frac{1}{\frac{1}{(1 - A_m) R_{0m} \Gamma_{\text{neutral}}} + \frac{1}{A_m^2 R_{0m} \gamma_m(\theta_{\text{im}}) \Gamma_{\text{ion}} + R_{\text{des},m}}} \quad (35)$$

where:

- $R_{\text{des},m}$ is the thermal desorption rate for material m (parameter `desorption_rate` in the `add_material` command).
- A_m is the anisotropy of material m (parameter `anisotropy` in the `add_material` command).
- R_{0m} is the etch rate on a flat surface of material m (parameter `rate` in the `add_material` command).

This model has the following properties:

- If one of the fluxes is zero, then the overall etch rate is zero since both neutrals and ions are required to etch the material.
- The etch rate becomes saturated when one component becomes too large relative to the other.

The neutral flux is evaluated as in the RIE2 and HDP2 models by considering the shadowing and the reemission probability on the surface. Ion reflections to the sidewalls can also be considered by setting the parameter `reflection`.

Wet Etching

Set `model=wet` in the `define_etch_machine` command to define a wet etching machine (see [define_etch_machine on page 242](#)).

This model assumes that the etchant concentration is constant at a specified distance above the top of the structure, and that the transport of the etchant to the surface of the structure occurs by diffusion. At the surface of the structure, the model assumes that the etchant is consumed by a first-order reaction.

Dry Etching

Set `model=dry` in the `define_etch_machine` command to define a dry etching machine (see [define_etch_machine on page 242](#)).

This model considers the combination of sputter etching and deposition processes. The etch process is induced by unidirectional high-energy ions that sputter the material of the structure (see [Ion-Milling on page 73](#)). At the same time, an LPCVD process is considered (see [Low-Pressure Chemical Vapor Deposition on page 65](#)).

The total deposition etch rate is evaluated as:

$$R_m = R_{\text{deposition}} \Gamma_{\text{neutral}} - H(x, y, z) R_{\text{ion-mill}, m} \gamma_m(\theta_{\text{im}}) \quad (36)$$

where:

- $R_{\text{deposition}}$ is the deposition rate on a completely flat surface (parameter `rate` in the `define_etch_machine` command).
- $R_{\text{ion-mill}, m}$ is the etching rate on a completely flat surface for material m (parameter `rate` in the `add_material` command).
- $H(x, y, z)$ is the function that accounts for the surface point shadowing as defined in [Equation 14 on page 64](#).

Crystallographic Orientation–Dependent Etching

Set `model=crystal` in the `define_etch_machine` command to define a crystallographic orientation–dependent etching machine (see [define_etch_machine on page 242](#)).

The etching rate is determined by the orientation of the exposed surface with respect to the lattice of its bulk material, which is assumed to be cubic. More precisely, the etching rate at any point of the exposed surface is computed as the spherical barycentric interpolation [7], along its normal direction, of the deposition rates along the $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ crystallographic directions (parameters `rate_100`, `rate_110`, and `rate_111` of the `define_etch_machine` command, respectively).

Compared to other built-in etching models, only one material (specified with the parameter `etchable_material` of the `define_etch_machine` command) can be etched using this model.

The crystallographic orientation of the material to be etched is expected to be set. If there are several regions with the material to be etched, their crystallographic orientations must be all set and they must be identical. See [Orientation-Dependent Models on page 56](#), [Setting Crystallographic Orientations on page 56](#), and [set_orientation on page 547](#).

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Level Set-Based Models

Simultaneous Etching and Deposition

Set `model=etchdepo` in the `define_etch_machine` command to define a simultaneous etching and deposition machine (see [define_etch_machine on page 242](#)).

This model considers the etching process due to sputtering induced by high-energy ions and the redeposition of this sputtered material. At the bottom of the trench, the polymer is usually removed by ion bombardment; while on the sidewalls, it accumulates forming a thin layer. This layer can inhibit the etching process.

The ion flux has an angular distribution $\cos^m \theta$, where m is set by the parameter `exponent`, or is a user-defined IAD (the parameter `iad`).

The deposition process is simulated considering that the incoming material flux $\Gamma_{\text{sputter deposition},i}$ at point i is the sum of the integrated sputtered flux $\Gamma_{\text{sputter},j}$, which is sputtered from point j and arriving at point i , plus the reemitted flux from all the visible points j :

$$\Gamma_{\text{sputter deposition},i} = \sum_{j \neq i} g_{ij} \Gamma_{\text{sputter},j} + (1 - \sigma) \sum_{j \neq i} g_{ij} \Gamma_{\text{sputter deposition},j} \quad (37)$$

Here, $\Gamma_{\text{sputter},j}$ is induced by the ion flux Γ_{ion} (see [Equation 7](#)).

Ion reflection at the sidewalls also can be considered by setting the parameter `reflection`. The angular distribution of sputtered material can be set with the parameters `sputter_type` and `exponent`.

Finally, the total rate is evaluated as:

$$R_m = R_{\text{deposition}} \Gamma_{\text{sputter deposition}} - R_{\text{etch, } m} \Gamma_{\text{sputter}} \quad (38)$$

where:

- $R_{\text{deposition}}$ is the deposition rate on a completely flat surface (parameter `rate` in the `define_etch_machine` command).
- $R_{\text{etch, } m}$ is the etching rate on a completely flat surface for material m (parameter `rate` in the `add_material` command).
- $\Gamma_{\text{sputter deposition}}$ is the indirect flux of sputtered material, as described in [Equation 37](#).

A positive total rate R_m indicates a net deposition; a negative total rate indicates a net etching.

Note:

In contrast to other models, in the `etchdepo` model, the sputter flux emitted from a point is set to zero if the sputter rate for the corresponding material is exactly zero. The sputter rate for a material can be zero either because it has been specified explicitly with the `add_material` command or because the properties of the material have not been specified with the `add_material` command.

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Level Set-Based Models

Simultaneous Etching and Deposition 2

Set `model=etchdepo2` in the `define_etch_machine` command to define a simultaneous etching and deposition 2 machine (see [define_etch_machine on page 242](#)).

This model considers the combined effect of etching in the ion-enhanced regime and the deposition due to polymerization. As in the ion-enhanced model, the ion flux removes the layer of atoms formed by the chemical reactions and damages the surface that favors chemical etching. The polymer deposits on the surface as in an LPCVD process and is removed with the ion-milling mechanism.

The etching due to ions is modeled as a sputter etching process, where the sputter yield function is defined as in [Equation 6](#).

The polymer also dissociates thermally, with a rate specified by the parameter `desorption_rate`. At the bottom of the trench, the polymer is usually removed by ion bombardment; while on the sidewalls, it accumulates forming a thin layer. This layer can inhibit the etching process. The etch rates and fluxes are evaluated as in the ion-enhanced model; while the polymer deposition rate is evaluated as in an LPCVD process.

The total deposition rate for all materials except the deposited material is:

$$R_m = R_{\text{deposition}} \Gamma_{\text{neutral depo}} - \frac{1}{\frac{1}{(1-A_m) R_{\text{etch},m} \Gamma_{\text{neutral etch}}} + \frac{1}{A_m R_{\text{etch},m} \gamma_m(\theta_{\text{im}}) \Gamma_{\text{ion}} + R_{\text{des},m}}} \quad (39)$$

The total deposition rate for the deposited material is:

$$R_m = R_{\text{deposition}} \Gamma_{\text{neutral depo}} - R_{\text{etch},m} \gamma_m(\theta_{\text{im}}) \Gamma_{\text{ion}} \quad (40)$$

where:

- $R_{\text{des},m}$ is the thermal desorption rate for material m (parameter `desorption_rate` in the `add_material` command).
- A_m is the anisotropy for material m (parameter `anisotropy` in the `add_material` command).
- $\Gamma_{\text{neutral etch}}$ is the total flux of neutrals, computed with a material-dependent sticking coefficient (specified with the `add_material` command). Its angular distribution can be specified with either the parameter `neutral_etch_exponent` or the `define_nad [species=neutral]` command.
- $\Gamma_{\text{neutral depo}}$ is the total flux of neutrals, computed with a material-independent sticking coefficient (specified with the `define_etch_machine` command). Its angular distribution can be specified with either the parameter `neutral_exponent` or with the `define_nad [species=neutral]` command.
- Γ_{ion} is the ion flux.

Void Modeling

This model considers surface diffusion and convection, which are added together to obtain the surface velocity. The surface diffusion term is based on the work of Sudoh *et al.* [14], which studied the evolution of Si when annealed in a H₂ atmosphere.

The void model implemented in Sentaurus Topography 3D addresses the imperfect filling of holes, where voids are formed, thereby preventing further filling. It is reasonable to assume that subsequent evolution is governed by the same diffusion processes, even if their rates might be quite different. In the Sudoh *et al.* paper (equation 2), surface diffusion is modeled as a function of the curvature K . The velocity of the surface is given by:

$$v = \frac{D_s \gamma \Omega^2 X_s}{kT} \frac{\partial^2 K}{\partial s^2} \quad (41)$$

where:

- D_s is the surface diffusivity.
- γ is the surface tension.
- Ω is the atomic volume.
- X_s is the number of atoms per unit surface area.

The convection term is needed to move the voids, as has been observed experimentally. In this model, convection is based on vacancy migration as described in [15]. In this paper, gradients in pressure drive the vacancy migration. In Sentaurus Topography 3D, it is assumed that vacancies attaching and detaching on opposite sides of a void cause void migration. According to [15], the current of vacancies is:

$$J \propto \nabla e^{\frac{-PV_0}{kT}} \quad (42)$$

where V_0 is the formation volume of the vacancy. The motion of the void is the opposite of the flow of vacancies, so that the total surface velocity becomes:

$$v = \frac{v_{0C}}{T} e^{\frac{-E_d}{kT}} \frac{\partial^2 K}{\partial s^2} - v_{0P} \vec{n} \cdot \nabla e^{\frac{-PV_0}{kT}} \quad (43)$$

where \vec{n} is the surface normal, $D_s = D_{s0} e^{\frac{-E_d}{kT}}$, and $v_{0C} \equiv D_{s0} \gamma \Omega^2 X_s / k$.

Spin-on-Glass Deposition Model

The `spin_on` model is used to determine the spin-on material profile over a given topographic substrate. The profile evolution of the film is computed by solving the Navier–Stokes equations under the lubrication theory for Newtonian fluids [8][9][10].

Given the initial thickness of the spin-on material (parameter `initial_thickness`), the profile evolution of the film is computed taking into account the capillarity and centrifugal forces acting on it. In addition, the film is supposed to evaporate during the process (parameter `evaporation_rate`). The spin-on material is characterized by its viscosity (parameter `viscosity`), its density (parameter `density`), and its surface tension with the surrounding fluid (parameter `surface_tension`).

The centrifugal force acting on the simulated structure is supposed to be constant over the simulation domain, and it is determined by the angular velocity of the wafer (parameter `angular_velocity`), the position of the simulated structure on the wafer (parameters `angular_position` and `radial_distance`), and the film density.

Reaction Models

Reaction models provide a very powerful and flexible means of describing the physical and chemical effects that occur on a wafer surface due to interaction with plasma species. Basic effects such as adsorption, reemission, sputtering, and chemical etching are described by surface reactions, using a syntax that is similar to that used for chemical reactions. Each reaction defines the interaction of a single gas-phase species with one or more surface species, along with the products that might result from this interaction. Reaction products can be emitted from the surface and eventually interact with other parts of the wafer surface, or they can be defined as being volatile, meaning that they have no effect in the simulation.

In the definition of a reaction model, unlike the definition of a level set–based model, there is no distinction between ion and neutral species. Indeed, a reaction model consists of a set of source species and a set of reactions. However, different properties (for example, angular distributions) can be assigned to each source species to effectively model both the neutral and the charged particles present in the reactor.

In addition, whereas for the level set–based models, the fluxes of the source species are always assumed to be normalized, reaction models require the specification of the absolute fluxes of the source species.

A reaction model is defined using the `define_model` command (see [define_model on page 289](#)). A source species is defined using the `add_source_species` command (see [add_source_species on page 203](#)); whereas, reactions are defined using the `add_reaction` command (see [add_reaction on page 182](#)).

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Feedback of Surface Reaction Products

The angular distribution of each source species can have an arbitrary shape and must be specified with the `define_species_distribution` command (see [define_species_distribution on page 337](#)). However, the angular distributions of the source species are not part of any model. Only when defining a machine with the `define_etch_machine` command, a reaction model is bound to the angular distributions of its source species (see [define_etch_machine on page 242](#)).

As detailed in [add_reaction on page 182](#), a reaction states a rule to transform a set of reactants into a set of products. Each reaction must contain one reactant species coming from the reactor, which must be either a source species or a species produced as a result of another reaction.

When the reactants become available, reactions are executed with a probability specified with the `add_reaction_properties` command (see [add_reaction_properties on page 188](#)). In the general case, the reaction probability depends on the angle between the traveling direction of the incoming species and the normal to the surface where the incoming species collides with the structure as well as on the energy of the incoming particle. The `define_probability` command allows you to define an energy-dependent and angle-dependent reaction probability (see [define_probability on page 299](#)). Since the execution of a reaction depends on a random decision, it is possible that no reaction occurs even if the reactants are available. When the reactants are available, but no reaction is actually executed, the incoming species is either stopped or reemitted in the reactor, as specified by the `default_event` parameter of the `define_species_properties` command (see [define_species_properties on page 355](#)).

Feedback of Surface Reaction Products

During a topography-processing step, a significant amount of surface reaction products is produced, which desorb from the wafer and interact with the plasma source [11]. In the following, these surface reaction products are referred to as *byproducts*.

A reaction model can include different types of plasma feedback interaction:

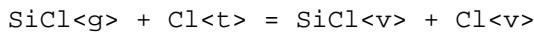
- Depletion of plasma radicals: The feedback of byproducts into the plasma leads to a consumption of plasma radicals (*loading effect*), which might result, for example, in a local decrease of the etch rate.
- Enhancement of plasma radicals: The feedback of byproducts triggers the emission of new plasma particles, which might lead, for example, to a local increase of the etch rate.

You can model both feedback effects, depletion and enhancement, in reaction models by defining feedback reactions at the plasma source (the *top plane* $\langle t \rangle$), which is located at a user-defined height above the substrate.

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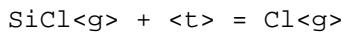
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To define a feedback reaction between a surface reaction product (for example, $\text{SiCl}_{<\text{g}>}$) and a plasma bulk species in the top plane (for example, $\text{Cl}_{<\text{t}>}$), you can define the following reaction:



This reaction corresponds to an annihilation of the plasma radical Cl , resulting in a decrease of the Cl concentration in the plasma bulk.

An enhancement of the particle flux emitted by the plasma source can be achieved by defining the following reaction:



where $<\text{t}>$ is a placeholder for *any* plasma bulk species. This reaction represents a generic reaction between an incoming surface reaction product ($\text{SiCl}_{<\text{g}>}$) and a plasma bulk species (represented by the placeholder $<\text{t}>$) at the top plane.

See [add_reaction on page 182](#), [add_reaction_properties on page 188](#), and [define_etch_machine on page 242](#) for details on the usage of the plasma feedback model.

Crystalline Materials, Nucleation, and Grain Growth

This section discusses crystalline materials, nucleation, and grain growth.

Defining Crystalline Materials

Crystalline and polycrystalline materials such as polysilicon are commonly used in modern industrial applications. While amorphous materials have a disordered atomic structure, crystals possess a highly symmetric and repeating pattern. In Sentaurus Topography 3D PMC, the only supported crystal structure is the diamond cubic lattice, which is the most common crystal structure in topography simulation applications.

Defining Monocrystalline Materials

To define a crystalline material, its lattice type, lattice constant, and orientation in space must be specified:

```
set_material_properties material=<c> type=crystalline \
    crystal_type=diamond flat_orientation=<v> \
    vertical_orientation=<v> [lattice_constant=<n>]
```

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The parameters `flat_orientation` and `vertical_orientation` are needed to define the orientation of the crystal lattice in space:

- `flat_orientation` sets the Miller indices of the crystal plane, which is perpendicular to the y-axis (wafer flat) of the wafer coordinate system.
- `vertical_orientation` sets the Miller indices of the crystal plane, which is perpendicular to the z-axis (vertical axis) of the wafer coordinate system.

Example 1 Define a structure consisting of crystalline silicon:

```
define_structure material=Silicon point_min={-1 -1 0} \
    point_max={3 1 10}

set_material_properties material=Silicon type=crystalline \
    crystal_type=diamond \
    flat_orientation={1 1 0} vertical_orientation={0 0 1}
```

Example 2 Set the crystal properties only for a subregion of the structure:

```
define_structure region=region1 material=Silicon \
    point_min={-1 -1 0} point_max={3 1 10}

set_material_properties region=region1 type=crystalline \
    crystal_type=diamond \
    flat_orientation={1 1 0} vertical_orientation={0 0 1}
```

Defining Polycrystalline Materials

Besides pure crystalline materials, polycrystalline materials can also be modeled, consisting of many small crystals (called crystallites or grains) of different orientations. You can specify the average size of the grains (parameter `average_grain_size`) as well as the preferred orientation, which is defined by a symmetry axis (`preferred_vertical_orientation`) and an angular spread around this axis (`vertical_orientation_spread`). The crystal grains are created randomly from the angular distribution around the preferred vertical orientation.

Example Create a polycrystalline region consisting of grains with an average size of 10 nm and a random crystal orientation around the preferred vertical direction:

```
set_material_properties region=region1 type=polycrystalline \
    crystal_type=diamond \
    preferred_vertical_orientation={0 0 1} \
    vertical_orientation_spread=10 \
    average_grain_size=10<nm>
```

For details about the syntax, see [set_material_properties on page 543](#).

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Crystalline Materials, Nucleation, and Grain Growth

Note:

For polycrystalline materials:

- The command `set_material_properties` converts the material properties of the structure at the time when it is called (similarly to the `filter_structure` command). It does not define material properties for materials that are created at a later time, for example, during a PMC deposition simulation (see [Adsorption and Deposition Reactions on page 88](#) for how to specify the crystal properties of PMC reaction products).
- If periodic boundary conditions are specified for the structure, then the generated grains are also periodic.

Loading and Saving Crystalline Materials From Files

When saving a structure to a TDR file, the morphology of the materials (amorphous, crystalline, or polycrystalline) and the crystal orientations are saved to the file as well. This allows you to reload the crystal properties when reading in the file.

Example 1 Save the crystal properties of silicon to a TDR file:

```
define_structure material=Silicon point_min={-1 -1 0} \
    point_max={3 1 10}

set_material_properties material=Silicon type=crystalline \
    crystal_type=diamond \
    flat_orientation={1 1 0} vertical_orientation={0 0 1}

save file=file1.tdr
```

Example 2 Load the crystal properties of silicon from the TDR file saved in Example 1:

```
define_structure file=file1.tdr
```

When saving a boundary structure, extracted from the PMC structure using the DC or VBE method, you can choose to save different crystal orientations as different regions. For details, see [save on page 521](#).

Note:

Crystal properties cannot be saved to the GC format (`save type=gc`).

Plotting Crystal Orientations

This section discusses how to plot crystal orientations.

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Boundary Structure (Using DC or VBE Method)

The easiest way to visualize the grains of polycrystalline materials is to save the structure with `save type=dc` or `save type=vbe`. You can also specify `grain_regions=true` to save each crystal orientation as a separate region in the output (see [Figure 16 \(left\)](#)). This makes it possible to color each crystal orientation independently:

```
save file=file1.tdr type=dc dc_version=2 grain_regions=true
```

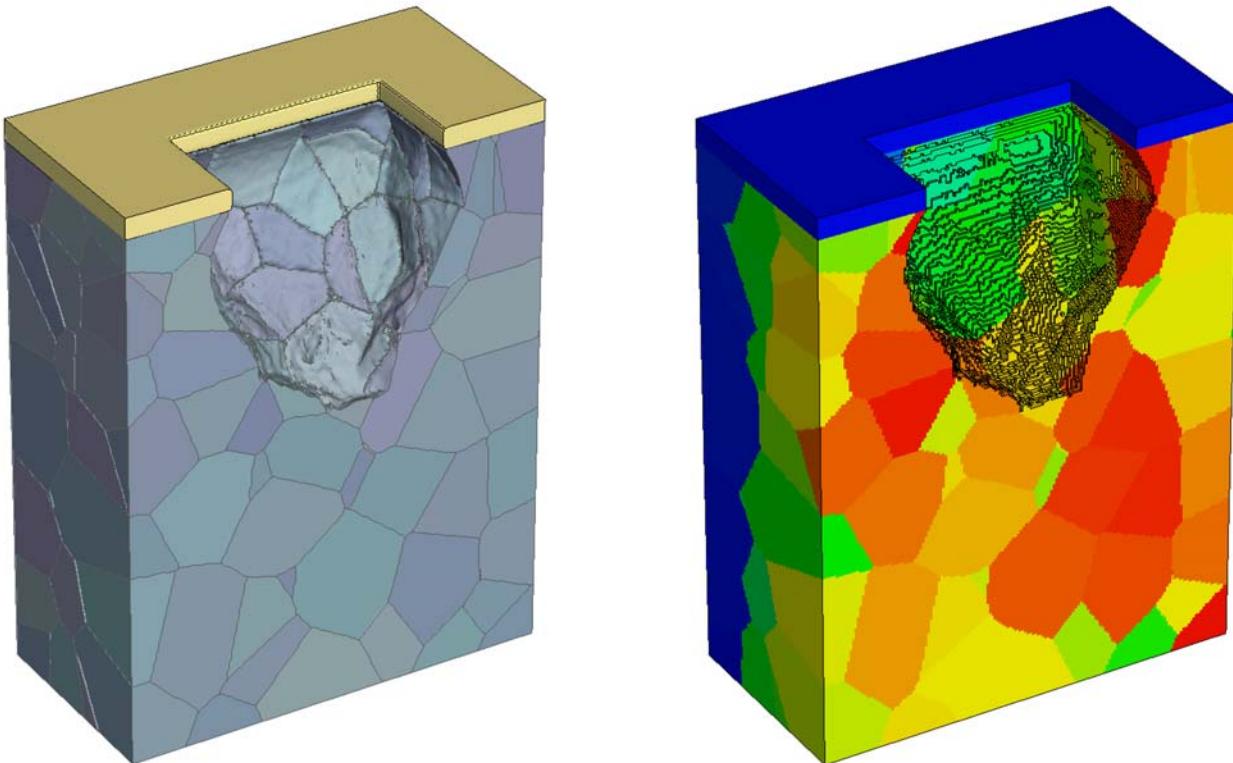
or:

```
save file=file1.tdr type=vbe grain_regions=true
```

Note:

When using the VBE method with `grain_regions=true`, only up to 240 different crystal orientations are supported (this corresponds to 240 grains in a structure).

Figure 16 (Left) Boundary structure containing polycrystalline material, with different grain orientations represented by different regions and (right) volume fraction plot (colors correspond to the solid number dataset)



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Volume Fraction Output

Another way to visualize crystal orientations is to write out the volume fractions:

```
save file=file1.tdr type=volume_fractions
```

This command creates a TDR file containing a dataset `solid_number` for each material in the structure. The solid number is a unique ID for each crystal orientation contained in the structure (`solid_number=0` is reserved for amorphous material). When plotting the solid number datasets in Sentaurus Visual, each crystal orientation will be shown in a different color (see [Figure 16 \(right\)](#)).

Crystal Orientation–Dependent Reactions

This section discusses reactions that are dependent on the crystal orientation.

Etching and Sputtering Reactions

In general, the etch reactivity on crystalline surfaces is affected by the crystal orientation of the exposed surface plane. To model crystal orientation–dependent effects, you can define crystal orientation–dependent reaction probabilities in the `add_reaction_properties` command.

Due to the symmetry properties of the crystal, it suffices to define the reaction probabilities on the main crystal planes. For example, for a diamond crystal, you must specify the reaction probabilities only on three independent planes (1 0 0), (1 1 0), and (1 1 1) (parameters `diamond_p_100`, `diamond_p_110`, and `diamond_p_111`). From those values, the reaction probabilities on all other surface planes (for example, (1 1 3), (2 1 3) ...) are computed by interpolation.

Example Consider a PMC etch model for crystalline silicon. The etch probability depends on the crystal orientation of the exposed surface and is specified for the three main crystal planes:

```
define_structure material=Silicon point_min={-1 -1 0} \
    point_max={3 1 10}
set_material_properties material=Silicon type=crystalline \
    crystal_type=diamond \
    flat_orientation={1 1 0} vertical_orientation={0 0 1}
.

.

.

define_model name=m description="Etching crystalline Silicon"
add_source_species model=m name=F
add_reaction model=m name=R expression="F<g> + Silicon<s> = Silicon<v>"
finalize_model model=m
.
```

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```
add_reaction_properties reaction=R p=1 diamond_p_100=1 \
diamond_p_110=0.7 diamond_p_111=0.1
```

Notes:

- In addition to the crystalline probabilities `diamond_p_i j k`, you must define the probability for amorphous surfaces `p`, since the structure might, in general, contain amorphous material as well.
- If more than one reaction is defined on the same surface material, then the sum of all probabilities must be less than or equal to 1 on each crystal plane:

$$\sum_{r \in \{\text{reactions with the same surface reactant}\}} p_{ijk, r} \leq 1 \quad \forall ijk \in \{(100), (110), (111)\}$$

- If the sum of the probabilities is less than one, then there exists a probability that no reaction is executed upon a surface collision. In that case, the default event is executed, which is defined in the `define_species_properties` command (see [define_species_properties on page 355](#)).

For details about the syntax, see [add_reaction_properties on page 188](#).

Adsorption and Deposition Reactions

This section describes adsorption and deposition of crystalline material on crystalline surfaces. For adsorption or deposition on amorphous substrates, see [Nucleation and Grain Growth on page 89](#).

To simulate the adsorption or deposition of material on a crystalline surface, you must specify whether the deposited layer is amorphous or crystalline by using the parameter `product_morphology` in the `add_reaction_properties` command:

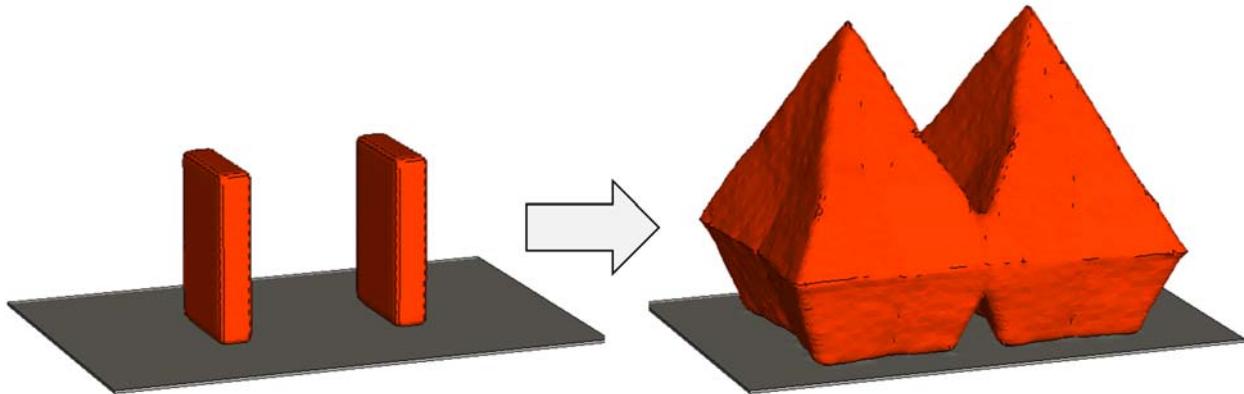
- To deposit amorphous material on a crystalline surface, set `product_morphology=amorphous`.
- To deposit crystalline material on a crystalline surface, adopting the same crystal orientation as the surface, set `product_morphology=same_as_surface_reactant`.

In analogy to etching and sputtering reactions, the probability for adsorption or deposition depends on the crystal orientation of the exposed surface plane. The resulting anisotropic deposition rates can lead to characteristic crystal shapes with sharp edges and facets (see [Figure 17](#)). To model orientation-dependent adsorption or deposition rates, you must provide the reaction probabilities on the main crystal planes (parameters `diamond_p_100`, `diamond_p_110`, and `diamond_p_111`).

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Crystalline Materials, Nucleation, and Grain Growth

Figure 17 Deposition on crystalline pillars: resulting shape shows characteristic sharp edges and facets



Example 1 Deposit crystalline PolySi on a (polycrystalline) PolySi surface, taking over the crystal properties (crystal type and orientation) of the surface:

```
define_model name=m description="Grain growth model"
add_source_species model=m name=Silane
add_reaction model=m name=R \
    expression="Silane<g> + PolySi<s> = PolySi<s> + PolySi<b>"
finalize_model model=m
.
.
.
add_reaction_properties reaction=R p=1 \
    product_morphology=same_as_surface_reactant \
    diamond_p_100=0.5 diamond_p_110=0.8 diamond_p_111=0.2
```

Example 2 Adsorb amorphous silicon a-Si on a polycrystalline PolySi surface:

```
define_model name=m description="Adsorption of amorphous Silicon"
add_source_species model=m name=Silane
add_reaction model=m name=R \
    expression="Silane<g> + PolySi<s> = a-Si<s>"
finalize_model model=m
.
.
.
add_reaction_properties reaction=R p=1 product_morphology=amorphous \
    diamond_p_100=0.5 diamond_p_110=0.8 diamond_p_111=0.2
```

Nucleation and Grain Growth

The adsorption or deposition of crystalline material (for example, polycrystalline silicon) on top of an amorphous substrate (for example, graphite) is commonly known as *crystal film growth*. In general, the morphology of the deposited film depends on the process conditions and can be amorphous (disordered), crystalline (oriented), or polycrystalline (multiple

Chapter 3: Model Descriptions

Crystalline Materials, Nucleation, and Grain Growth

grains). Crystal film growth is a complex physical process that consists of many simultaneous atomistic effects, including adsorption, desorption, nucleation, grain growth, and coalescence (see, for example, [13], Chapter 8.5).

You can use a simplified model to describe crystal film growth by using only two parameters (see [Figure 18](#)):

- The parameter `p_nucleation` sets the probability that a gaseous reactant sticks stably to the surface (and, therefore, becomes a so-called adatom). This probability implicitly describes the net effect of the atomistic processes of adsorption, desorption, and nucleation. By default, the crystal type of the deposited nucleus is diamond, and the crystal orientation is chosen randomly by the simulator.
- The parameter `p_island_growth` sets the probability that a new gaseous reactant, which is adsorbed near an existing grain, attaches to that grain. This parameter implicitly describes adatoms sticking to the boundary of grain islands.

Example Grow a crystalline PolySi film on an amorphous graphite substrate (see [Figure 18](#)):

```
define_model name=m description="Nucleation and grain growth model"
add_source_species model=m name=Silane
add_reaction model=m name=R \
    expression="Silane<g> + Graphite<s> = PolySi<s> + Graphite<b>"
finalize_model model=m
.
.
.
add_reaction_properties reaction=R p=1 \
    product_morphology=crystalline crystal_type=diamond \
    p_nucleation=1e-6 p_island_growth=1
```

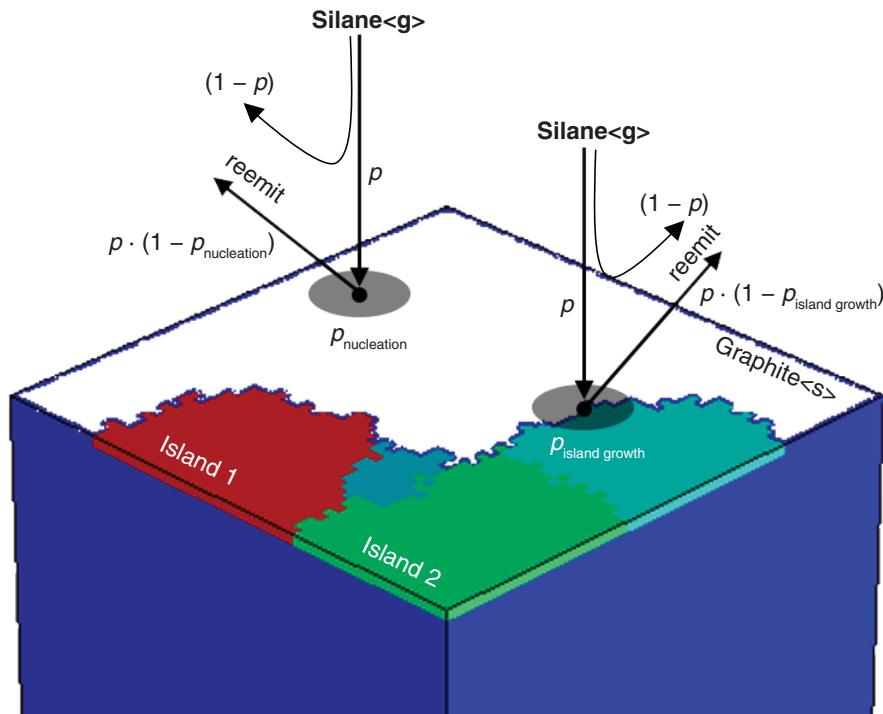
Notes:

- You can use `product_morphology=crystalline` only together with a nucleation model, that is, together with the nucleation parameters `p_nucleation` and `p_island_growth`.
- The probability of nucleation is typically orders of magnitude smaller than the probability of island growth. This is explained by the underlying atomistic processes: The probability of an adatom forming a new stable island is much lower than the probability of it sticking to a preexisting island. The ratio of `p_nucleation` to `p_island_growth` determines how many grains are deposited on the surface; therefore, you can control the average grain size by varying these parameters.
- After some time, the entire surface will be covered by a thin film of grains. To further grow these grains in height, you need to define a deposition reaction (see [Adsorption and Deposition Reactions on page 88](#)).

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Diffusion

Figure 18 Nucleation and grain growth model: If Silane $\langle g \rangle$ hits the amorphous Graphite $\langle s \rangle$ surface in a free area, a new crystal nucleus with a random crystal orientation is created with probability $p \cdot p_{\text{nucleation}}$ (where p is the overall probability that the reaction is executed). On the other hand, if Silane $\langle g \rangle$ hits the Graphite $\langle s \rangle$ surface near an existing PolySi $\langle s \rangle$ island, it attaches to that island with probability $p \cdot p_{\text{island growth}}$, taking over the crystal properties of the island. If no nucleation or attachment occurs, then Silane $\langle g \rangle$ is reemitted or discarded (depending on the default event defined for Silane $\langle g \rangle$).



Diffusion

Surface diffusion is available for deposition reactions and can be specified separately for each reaction, using the `add_reaction_properties method=diffusion` command. The implementation uses the random walk method to model diffusion. The following methods are implemented:

- Choose the **pure random walk** method (`biased_random_walk=last_step`) to model a pure random walk with a fixed number of steps given by parameter `num_diffusion_steps`.
- Choose the **biased random walk** method (`biased_random_walk=always`) to model the effects of energetic barriers such as surface roughness. The number of executed diffusion steps might be less than `num_diffusion_steps`, depending on the surface roughness.

Chapter 3: Model Descriptions

Surface Transport Model

Example

Specify that the silane particle, after hitting the surface, will execute a five-step random walk along the surface until it reaches a suitable surface site to which to stick:

```
define_model name=m \
    description="Surface diffusion of PolySi on Graphite"
add_source_species model=m name=Silane
add_reaction model=m name=R \
    expression="Silane<g> + Graphite<s> = PolySi<s> + Graphite<b>"
finalize_model model=m
.
.
.
add_reaction_properties reaction=R p=1 method=diffusion \
    biased_random_walk=always num_diffusion_steps=5
```

There are additional numeric parameters to control the algorithm to minimize surface roughness (see [add_reaction_properties on page 188](#)). These parameters are set to reasonable default values.

Surface Transport Model

Particles impinging a structure are not always reemitted or attached to the impingement site. They can also be physically adsorbed (*physisorbed*) and can form adatoms that diffuse on the surface. These diffusing adatoms can either react with the material on the surface or desorb into the gas.

The surface transport model simulates the diffusion of adatoms on the surface of a structure and the deposition, nucleation, crystal growth, and desorption of these diffusing particles. This model can simulate the formation of nuclei on a substrate material and the subsequent crystalline growth of these nuclei.

The surface transport model works as follows: first, a gas particle is physisorbed on the surface to form an adatom. Second, the model defines which subprocess types, or events, the adatom can undergo. You define the set of possible events for each adatom on each surface material by using the `add_event` command (see [add_event on page 153](#)).

The surface transport model supports the following events: adsorption, deposition, surface diffusion, nucleation, attachment (grain growth), and desorption. The likelihood of an event is controlled by the `r` parameter. For a diffusion event, instead of a rate, you can specify a diffusivity. For each adatom species, you must define a list of events to specify which events are possible on which surface material.

The reaction of the surface particle (the event) is decided while the particle travels on the surface and, therefore, depends on the underlying substrate material, as opposed to diffusion described in [Diffusion](#), in which the reaction is executed when the gas particle

Chapter 3: Model Descriptions

Surface Transport Model

impacts the surface and, only thereafter, the reaction product can diffuse on the surface of the substrate.

Example

```
define_model name=m description= \
    "Surface diffusion model with nucleation and grain growth"
add_source_species model=m name=A

## Create a diffusing adatom (tag <a>)
add_reaction model=m name=r1 expression="A<g> + B<s> = A<a> + B<s>"
finalize_model model=m
...

## Define a transport model
define_surface_transport_model name=M

## Diffusion: define diffusion events for adatom A on surface material B
add_event type=diffusion model=M species=A material=B diffusivity=0.01

## Desorption: the desorbed gaseous particle is reemitted as A<g>
add_event type=desorption model=M species=A material=B model=M \
    r=1e8 tracked=true product=A

## Deposition: the diffusing species A is deposited as species B
## on surface material B
add_event type=deposition model=M species=A material=B r=1e9 \
    type=deposition product=B

## Form a new crystal nucleus of species C (with a random crystal
## orientation)
add_event type=nucleation model=M species=A material=B r=1e7 \
    crystal_type=diamond product=C

## Grain growth, that is, diffusion on surface material B to a grain
## boundary and attachment to crystalline species C (taking on the
## crystal orientation of C)
add_event type=attachment model=M species=A material=B grain=C \
    diamond_r_100=1e9 diamond_r_110=2e9 diamond_r_111=5e9

## Crystal growth, that is, deposition on a crystal of species C
## (defined by the crystal orientation of C)
add_event type=deposition model=M species=A material=C product=C \
    diamond_r_100=1e9 diamond_r_110=2e9 diamond_r_111=5e9
...
define_etch_machine model=m surface_transport_model=<c>
```

Damage Modeling in PMC Simulations

Subsurface damage has been observed during plasma etching for many different material systems. This damage is attributed to high-energy ions impacting the surface during the etching process, resulting in various changes to the damaged material such as amorphization of crystalline materials, formation of dangling bonds, and mixing of atoms and materials.

Analytic Damage Modeling

A simple analytic model is available to track this damage, which increments a damage field with a Gaussian pulse for each ion impact. This model is based on the Hobler damage model [16] and can be specified for any combination of incoming ion and target material.

The addition of each ion results in the damage field being incremented by the following formula, where y is the primary direction, and x_1 and x_2 are the lateral directions:

$$\begin{aligned} f_{\text{damage}} &= f_p(y) \times f_l(x_1, x_2) \\ f_p(y) &= \frac{\text{total_damage}}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y - R_p)^2}{2\sigma^2}} \\ f_l(x_1, x_2) &= \frac{1}{2\pi\sigma_l^2} e^{-\frac{x_1^2 + x_2^2}{2\sigma_l^2}} \end{aligned} \tag{44}$$

where:

- R_p is the peak of the profile and is given by the parameter `projected_range`.
- σ is the spread of the profile in the primary direction and is given by the parameter `sigma`.
- σ_l is the spread of the profile in the lateral direction and is given by the parameter `lateral_sigma`.
- `total_damage` is the integral of damage over all space.

For details, see [define_damage on page 217](#).

The damage field can be stored in a TDR file by using the `save type=transfer` command. Sentaurus Visual can read this file to visualize the structure. An integral of the damage is available through the `extract type=damage_integral` command. The integration domain can be limited with the parameters `point_min` and `point_max`.

Damage Modeling With Binary Collision Approximation

To compute the damage produced, a detailed modeling of the ion-solid interaction based on the binary collision approximation (BCA) model has been introduced as a special type of PMC reaction – *BCA reaction*. At the core of the algorithm is a two-body (that is, binary) collision of two atoms.

The model considers the impact of the collision as well as the mass and atomic number of both species and includes electron stopping. BCA reactions are based on previous work in sputtering and ion implantation [16][17][18].

The PMC method tracks ions through the gas until they hit the structure. A BCA reaction consists of one incoming “source” species and multiple target species and, if the BCA reaction has been created for the combination of ion species and material type, then the BCA model computes the interaction between the ion and material species, imparting some of the energy of the ion to the material particle, potentially creating a recoil and leaving behind a vacancy. The trajectories of recoils are followed during subsequent collisions, and the collection of recoils and vacancies produced are called a cascade. Recoils with enough energy that are directed out of the solid are considered to be sputtered, and these particles are then either tracked through the gas or discarded.

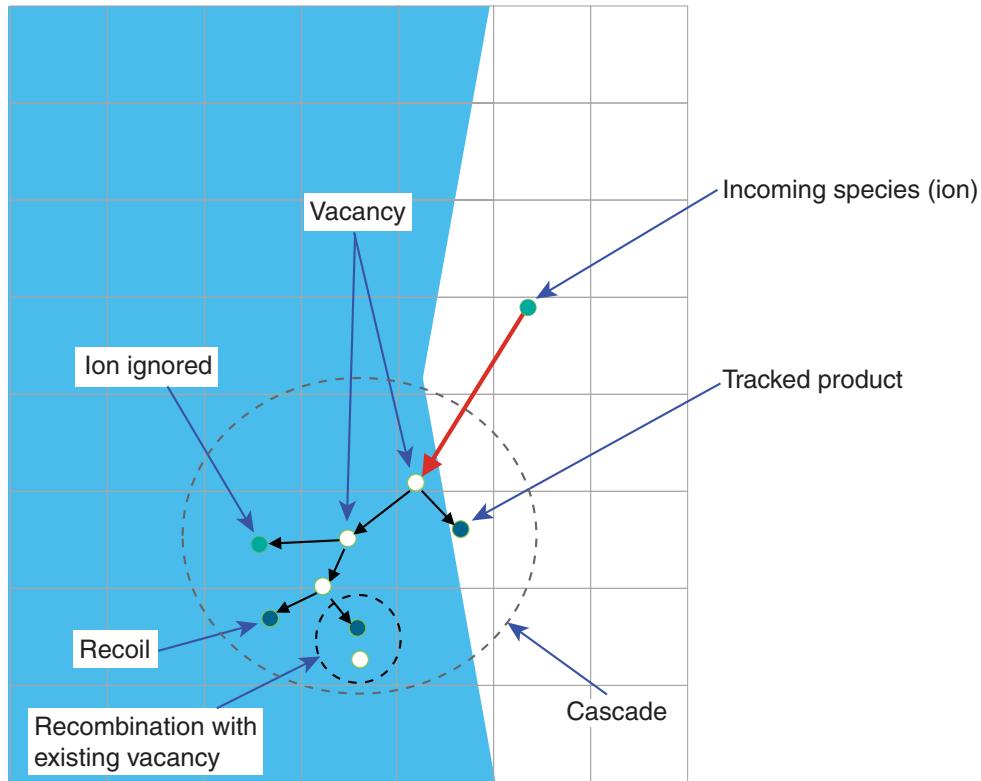
BCA Reactions

Similar to standard PMC reactions, the `add_reaction` command is used to specify BCA sputtering if `type=bca` is given in the specification. In addition, related specifications are required for BCA reactions in the `define_species_properties` and `add_source_species` commands.

For collisions involving the specified reactants, the probability of a BCA reaction occurring is handled in the same way as for other reactions. This allows for mixing BCA reactions with non-BCA PMC reactions.

As previously mentioned, the probability of the reaction occurring refers to the probability that the BCA model should be invoked. When invoked, the BCA model computes a full cascade, determining the types and numbers of emitted particles.

Figure 19 Schematic of a BCA cascade with the reaction species



BCA Damage Model

The damage is updated after the BCA model computes a cascade and is defined as follows:

$$\text{Damage} = \frac{r + v}{2} \quad (45)$$

where r is the recoil volumetric density and v is the vacancy volumetric density.

The fields `recoil` (r) and `vacancy` (v) are stored in the PMC structure. When a PMC structure is created, `recoil` and `vacancy` are initialized to 0 and are computed automatically when BCA reactions are active. The values can be viewed by saving a volume fractions file by using `type=volume_fractions` in the `save` command. Subsequent PMC steps with active BCA reactions will increment the damage starting from the stored values.

Damage Recombination

For high concentrations of damage, the probability of vacancies and recoils recombining can become significant. In other words, when a recoil has lost all its energy, it might be close enough to a vacancy to fill it, removing a v and an r from the cell.

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References

To model this effect, the concept of recombination length is introduced, which can be specified by using the `recombination_length` parameter of the command `define_species_properties`. This material-dependent parameter is computed for each cell according to the material composition of the cell.

This parameter sets an interaction volume by using $4\pi r^3/3$, where r is the recombination length. Specifying `recombination_length=0` switches off recombination.

User-Defined Damage Initialization

By default, the fields `recoil` and `vacancy` are initialized to 0. You can use the `set_field` command to set the value of the `recoil` and `vacancy` fields of a PMC structure (see [set_field on page 542](#)).

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4

Plasma Modeling

This chapter describes plasma modeling in Sentaurus Topography 3D.

Simulation Modules

A plasma model consists of two simulation modules: a global plasma bulk model and a sheath model.

The plasma bulk model computes the ion, neutral, and electron densities and the electron temperature in the plasma bulk region for given plasma equipment parameters, such as RF power, pressure, and inlet gas flows.

The sheath model takes as input the species densities and the electron temperature computed by the plasma bulk model, as well as the electrode parameters (such as RF bias power, RF bias voltage, and RF bias current), and computes the energy and angular distributions of the ions and neutrals impinging on the wafer surface.

User Input Flow

[Figure 20](#) shows the input flow of a plasma model.

You create a plasma model by using the `define_plasma_model` command, which sets the bulk and sheath model types to be used for the plasma simulation (see [define_plasma_model on page 298](#)).

In addition, a plasma model consists of a set of neutral and ion species, and a list of reactions between them. You can add species to the model by using the `add_species` command (see [add_species on page 205](#)). Reactions between species are added by using the `add_bulk_reaction` command (see [add_bulk_reaction on page 149](#)).

Note:

All species names occurring in reaction expressions must have been previously defined in the `add_species` command.

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User Input Flow

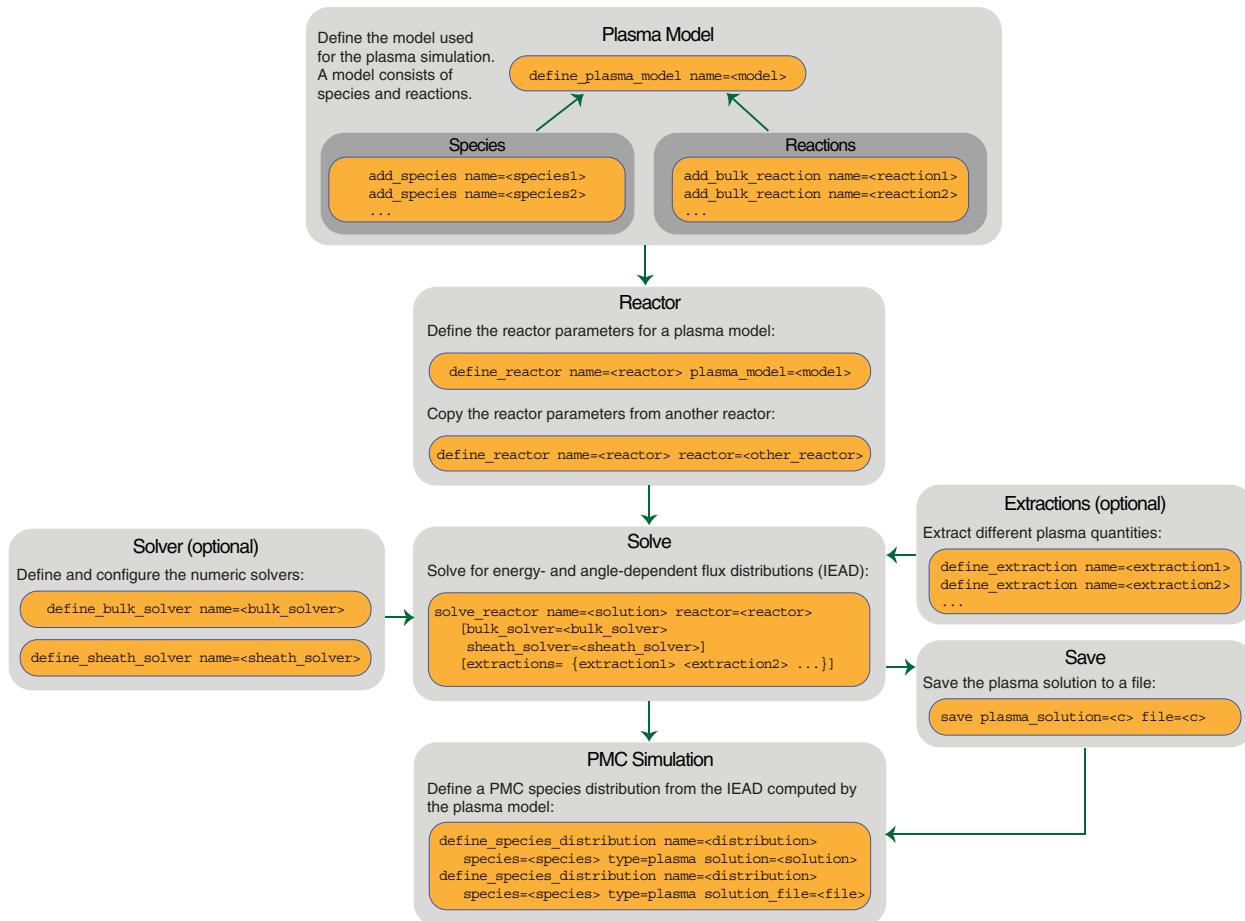
For example:

```
define_plasma_model name=M bulk_model_type=global \
sheath_model_type=circuit

add_species plasma_model=M name=Ar  mass=39.948<amu> charge=0
add_species plasma_model=M name=Ar+ mass=39.948<amu> charge=+1

add_bulk_reaction plasma_model=M name=r \
expression="Ar + e- = Ar+ + 2e-" \
rate_coefficient_type=arrhenius a=2.3e-14 b=0.6329 c=16.0627 \
energy_transfer=15.76<eV>
```

Figure 20 Input flow of a plasma model



The reactor parameters (such as power, gas flow, and pressure) to be used in the simulation must be specified in the `define_reactor` command (see [define_reactor on page 301](#)). Reactor parameters can also be initialized as a copy from another reactor object (see the

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User Input Flow

following `solve_reactor` example). When initializing a reactor from another reactor, you can modify specific reactor parameters in the same command. For example:

```
define_reactor name=R plasma_model=M type=icp radius=15<cm> \
    height=8<cm> power=1000<W> pressure=10<mTorr> \
    inlet_gas_flow= {{Ar 40<sccm>}} gas_temperature=400<K> \
    rf_bias_frequency=3.6<MHz> rf_bias_power=40<W>

define_reactor name=R2 reactor=R

define_reactor name=R3 reactor=R power=500<W> gas_temperature=300<K>
```

Finally, the plasma simulation is executed by the `solve_reactor` command, which computes the energy- and angle-dependent flux distributions of the species defined in the plasma model (see [solve_reactor on page 548](#)). The energy-angular flux distributions can be used directly in a PMC simulation, or they can be saved to a file. You can define a PMC species distribution directly after the plasma simulation by calling `define_species_distribution` with the name of the plasma solution (as specified in the `solve_reactor` command), or you can load the distribution from a file containing the plasma solution.

Example 1

```
solve_reactor name=S reactor=R

define_species_distribution name=sd species=Ar+ type=plasma solution=S
```

Example 2

```
solve_reactor name=S reactor=R

save type=plasma solution=S file=solution.plasma

define_species_distribution name=sd species=Ar+ type=plasma \
    solution_file=solution.plasma
```

If you want to analyze the plasma simulation further, then you can extract different dataset types such as the species densities in the plasma bulk, the electron temperature, the reaction statistics in the plasma bulk, the convergence residuals, the electron energy distribution, and the sheath characteristics (potential waveform, sheath currents, sheath capacitance, flux, electric field, and so on). You can define several extraction quantities by calling the `define_extraction` command multiple times with different names (see [define_extraction on page 252](#)). Finally, you must pass a list of extraction names to the `solve_reactor` command. For example:

```
define_extraction name=ex1 type=plasma bulk_model_type=global \
    quantities={state residuals reactions}

define_extraction name=ex2 type=plasma sheath_model _type=circuit \
    quantities={energy_distribution wall_potential sheath_width}
```

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Plasma Bulk Model

...

```
solve_reactor name=S reactor=R extractions={ex1 ex2 ... }
```

For a complete list of the available extraction quantities, see [Table 37 on page 271](#).

Optionally, you can configure the numeric solvers used to compute the solution in the `solve_reactor` command. The bulk solver can be configured by calling the command `define_bulk_solver`, and the sheath solver is specified in the `define_sheath_solver` command. If you do not specify a solver explicitly, the default solvers are used (see [define_bulk_solver on page 210](#) and [define_sheath_solver on page 330](#)).

Plasma Bulk Model

The plasma bulk model describes the complex physical processes in the plasma bulk region, which is governed by reactions between electrons and gas particles. Depending on the operating conditions of the plasma reactor (such as applied power and pressure), high-energetic collisions between plasma particles are triggered, producing energetic ions and other byproducts. At the boundary of the plasma bulk region, ions escape into the sheath region at a certain rate, where they are accelerated by the sheath potential towards the structure.

The main characteristics of the plasma bulk region are described by particle densities and the electron temperature. In the global plasma bulk model, the plasma species in the reactor are assumed to be well mixed, such that the species densities and temperatures can be treated as spatially uniform.

You can use the global plasma bulk model by setting `bulk_model_type=global` in the `define_plasma_model` command (see [define_plasma_model on page 298](#)).

Particle Density and Energy Balance

Unless otherwise stated, the input parameters mentioned in this section refer to the command `define_reactor` (see [define_reactor on page 301](#)).

The governing equations of the plasma bulk model are the particle continuity equations for the species densities and the energy conservation equation for the electron temperature.

The continuity equation for the i -th species is given by [1][2]:

$$\frac{\partial n_i(t)}{\partial t} = R_{\text{gain}, i}(t) - R_{\text{loss}, i}(t) + Q_{\text{inlet}, n} - n_i(t)Q_{\text{outlet}}(t) - n_i(t)v_{\text{loss}, i}(t) \quad (46)$$

Chapter 4: Plasma Modeling

Plasma Bulk Model

where:

- t denotes the time.
- $n_i(t)$ is the volume-averaged particle number density of species i .
- $R_{\text{gain}, i}(t)$ is the density increase by production of species i in the reactions. The total density gain rate by all reactions is given by:

$$R_{\text{gain}, i}(t) = \sum_{r \in \{\text{reactions}\}} R_{\text{gain}, i, r}$$

where $R_{\text{gain}, i, r}$ is the density gain rate by reaction r :

$$R_{\text{gain}, i, r} = \begin{cases} R_r, & \text{if species } i \text{ is a product of reaction } r \\ 0, & \text{else} \end{cases} \quad (47)$$

and the reaction rate of reaction r is:

$$R_r = k_r(T_e) \prod_{j \in \{\text{reactants of } r\}} n_j \quad (48)$$

Here:

- $k_r(T_e)$ denotes the rate coefficient associated with reaction r , which depends on the electron temperature T_e .
- n_j are the reactant densities of reaction r .
- $R_{\text{loss}, i}(t)$ is the density decrease by consumption of species i in the reactions. The total density loss rate by all reactions is given by:

$$R_{\text{loss}, i}(t) = \sum_{r \in \{\text{reactions}\}} R_{\text{loss}, i, r}$$

where $R_{\text{loss}, i, r}$ is the density loss rate by reaction r :

$$R_{\text{loss}, i, r} = \begin{cases} R_r, & \text{if species } i \text{ is a reactant of reaction } r \\ 0, & \text{else} \end{cases}$$

- $Q_{\text{inlet}, n}$ is the source term by the gas inlet (specified by the `inlet_gas_flow` parameter).
- $Q_{\text{outlet}}(t)$ is the loss term by the gas outlet.

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Plasma Bulk Model

- $v_{\text{loss}, i}(t)$ is the loss rate of species i escaping into the sheath at the plasma bulk boundary.

All quantities in [Equation 46](#) are spatially averaged over the volume of the plasma bulk.

The plasma bulk is modeled as a cylindrical region of radius R_{bulk} (parameter `radius`) and height L_{bulk} (parameter `height`) in the inner of the plasma chamber. As suggested in [\[3\]](#), the effective dimensions R_{bulk} and L_{bulk} of the plasma bulk are related to the actual dimensions of the plasma chamber R and L by the scaling factors h_R and h_L :

$$\begin{aligned} R_{\text{bulk}} &= R \cdot \sqrt{h_L} \\ L_{\text{bulk}} &= L \cdot \frac{h_R}{\sqrt{h_L}} \end{aligned} \quad (49)$$

The scaling factors h_R and h_L depend on the mean free path λ of the ions:

$$h_R = 0.8 \left(4 + \frac{R}{\lambda} \right)^{-0.5}$$

$$h_L = 0.86 \left(3 + \frac{L}{2\lambda} \right)^{-0.5}$$

These factors reduce to $h_R = 0.4$ and $h_L = 0.5$ in the collisionless limit, which is suitable for inert gases [\[4\]](#).

The total pressure is computed by the thermodynamic relation [\[4\]](#):

$$p(t) = \sum_{\substack{i \in \text{ion} \\ \text{and neutrals}}} n_i(t) k_B T_{\text{gas}} \quad (50)$$

where:

- The sum runs over all ions and neutral species.
- $n_i(t)$ is the density of species i .
- k_B is the Boltzmann constant.
- T_{gas} denotes the gas temperature, specified by the `gas_temperature` parameter.

The pressure inside the plasma chamber remains constant at the user-specified value in the `pressure` parameter. This is done by a pressure controller, which automatically calibrates the pumping speed at the outlet, such that the total pressure remains at the user-defined fixed value. The characteristic retardation of the pressure controller can be adjusted by the parameter `pressure_relaxation_time`.

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Plasma Bulk Model

To prevent nonphysical negative values, reasonable lower cutoff values are defined for all solution variables (ion, neutral and electron density, and electron temperature). You can adjust these values by using the parameters `min_density`, `min_electron_density`, `min_electron_energy`, and `min_density_relaxation_time`.

A key assumption in the modeling of the plasma bulk region is the charge-neutrality condition. Since the number of positively charged particles in the plasma bulk region is assumed to equal the number of negatively charged particles, the total charge equals zero.

For the electron density $n_e(t)$, this implies [5]:

$$n_e(t) = \sum_{i \in \text{ions}} q_i \cdot n_i(t) \quad (51)$$

where q_i is the charge of ion i , measured in units of the unit charge e .

To ensure the correct treatment of the energy balance in the plasma bulk region, the model simultaneously solves a power balance equation, given by [1][3][6][7]:

$$P_{\text{abs}} = P_e(t) + P_{\text{reaction}}(t) + P_{\text{loss}}(t) \quad (52)$$

where:

- P_{abs} is the total power absorbed by the system. The total absorbed power is assumed to be proportional to the time average of the RF power applied to the reactor (specified by the `power` parameter):

$$P_{\text{abs}} = \alpha \langle P_{\text{rf}}(t) \rangle_t$$

where $\alpha \in [0, 1]$ is the power absorption coefficient (specified by the parameter `power_absorption_coefficient`).

- $P_e(t)$ is the power absorbed by the bulk electrons.
- $P_{\text{reaction}}(t)$ is the power transferred in plasma bulk reactions.
- $P_{\text{loss}}(t)$ is the power lost into the reactor walls.

When calling the `solve_reactor` command, the governing equations (Equation 46, Equation 50, Equation 51, and Equation 52) are solved simultaneously until a stationary state is reached. The initial values for the species densities and the electron temperature are found automatically. However, you can define your own initial values by using the `density` and `electron_temperature` parameters.

Bulk Reactions

The plasma bulk model supports user-defined plasma bulk reaction sets. Bulk reactions can be defined by the `add_bulk_reaction` command, which takes the reaction equation, the

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reaction rate, and the energy transferred during the reaction (see [add_bulk_reaction](#) on page 149).

The reaction equation (specified by the `expression` parameter) consists of two reactant species, and one or more reaction products. For example:

```
expression= "Ar + e- = Ar+ + 2e-"
```

While no stoichiometric coefficients other than 1 are allowed on the reactant side, the stoichiometric coefficients of the reaction products can be arbitrary positive integers.

The rate at which each reaction is executed in the plasma bulk region is specified by a rate coefficient $k_r(T_e)$. The rate coefficient depends on the electron temperature T_e by either an Arrhenius law (`rate_coefficient_type=arrhenius`):

$$k_r(T_e) = a \cdot \left(\frac{T_e}{T_{\text{ref}}}\right)^b \cdot \exp\left(-\frac{c}{T_e}\right) \quad (53)$$

or a generalized Arrhenius law (`rate_coefficient_type=general_arrhenius`):

$$k_r(T_e) = \exp\left(a + b \ln T_e + \frac{c}{T_e} + \frac{d}{T_e^2} + \frac{e}{T_e^3} + f \cdot T_e + g \cdot T_e^2\right) \quad (54)$$

where the coefficients a , b , c , d , e , f , and g are listed in reaction tables (for example, see [2][8]).

In the previous example reaction, an Ar neutral is transformed into an Ar⁺ ion. During this reaction, the density of Ar reduces by an amount proportional to $n_{\text{Ar}} n_e k_r(T_e)$, while the density of Ar⁺ increases by the same amount.

In addition, a certain amount of energy is consumed by this reaction, which is specified by the `energy_transfer` parameter. By convention, the energy transfer is positive for endothermal reactions and negative for exothermal reactions. Accordingly, the amount of energy consumed or produced by reactions leads to a decrease or an increase of the electron temperature by the power balance equation ([Equation 52](#)).

You can save and plot a rate coefficient, which you defined using the `add_bulk_reaction` command (see [add_bulk_reaction](#) on page 149), as a function of the electron temperature, by calling the `save plasma_model=<c> quantity=rate_coefficient` command (see [save](#) on page 521).

Extracting Bulk Datasets

You can further analyze the plasma bulk simulation by saving and plotting various physical datasets.

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By calling the `define_extraction type=plasma bulk_model_type=global quantities=<1>` command, you can extract:

- `quantities=electron_energy_distribution`: The steady-state energy distribution $\varepsilon_e(E)$ of the electron in the bulk
- `quantities=reactions`: The reaction rate R_r (see [Equation 48](#)) of each bulk reaction r as a function of time
- `quantities=residuals`: The convergence residuals of the solution variables n_i , n_e , and T_e in [Equation 46](#), [Equation 51](#), and [Equation 52](#) as a function of time
- `quantities=species_balance`: For each species i , the time-averaged rate of production (or consumption) in each reaction r (see [Equation 47](#)):

$$\Delta R_{i,r} = \int_0^T (R_{\text{gain},i,r} - R_{\text{loss},i,r}) dt$$

- `quantities=state`: The ion or neutral densities n_i , the electron density n_e , the electron temperature T_e , the electron energy density $\varepsilon_e = 3/2n_e T_e$, the pressure p , and the absorbed power P_{abs} as a function of time
- `quantities=waveforms`: When simulating pulsed powers: The periodic steady-state waveforms of the ion or neutral densities n_i , the electron density n_e , the electron temperature T_e , and the absorbed power P_{abs} as a function of time for one period of the power pulse

The time-dependent quantities can be written to a file at regular time intervals (parameter `file_update_step`) while the simulation is still running. You can also define the sampling rate at which the data points are measured (parameter `time_step` or `extraction_step`). The datasets can be written to a TDR file (`output_type=tdr`) or to a CSV file (`output_type=csv_file`) or both files. You can reduce the number of datasets written by applying filters to the set of species names or reaction equations (parameters `species`, `species_pattern`, `reactions`, and `expression_pattern`). See [define_extraction on page 252](#) for details.

Source Power Pulsing

The latest plasma reactors support not only single-frequency RF biasing, but also dual and triple frequencies (for example, 60 MHz, 10 MHz, 2 MHz), to better control energetic ion bombardment onto the wafer. While the low frequency controls the shape of the ion energy distribution, the high frequency affects the level of ionization in the plasma bulk and can result in a modulation of the ion energy distribution [\[9\]](#).

Bulk Simulation With Pulsed Power

To simulate power pulsing, you can define a time-dependent function expression for the source power (parameter `power_waveform` in the `define_reactor` command; see

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[define_reactor on page 301](#)). The power function is assumed to be periodic in time with a period given by the parameter `power_period`. By default, the power function is sampled using 100 points per period, which can be changed by using the `num_waveform_samples` parameter.

For information about the syntax for function expressions, see [Syntax for Expressions on page 139](#).

Example 1 Set the input power to a square pulse with an on-value of 2000 W, an off-value of 200 W, a period of 1 ms (corresponding to a pulse frequency of 1 MHz), and a duty ratio of 20%:

```
define_reactor ... \
    power_waveform="square_pulse( t<s>, 2000, 200, 1e-6, 0.2 )" \
    power_period=1e-6<s>
```

Example 2 Set the input power to a sinusoidal wave with a DC power of 1600 W, an amplitude of 400 W, and a frequency of 1 MHz (corresponding to a period of 1 ms):

```
define_reactor ... power_waveform="1600 + 400*sin(2*M_PI*1e6*t)" \
    power_period=1e-6<s>
```

Tip:

To improve convergence when simulating pulsed powers, it is advisable to not start the bulk simulation from scratch, but to initialize the plasma state (densities and electron temperature) from the solution of an equivalent continuous-wave power simulation using the time-averaged power.

To initialize the state from a previous solution, see the `solution` or `solution_file` parameter in the `define_reactor` command (see [define_reactor on page 301](#)).

When solving a plasma model with a pulsed power waveform, the steady-state species densities and the electron temperature are periodic waveforms. The waveforms can be saved and visualized by defining an extraction with `type=plasma` and `quantities=waveforms` (see [define_extraction on page 252](#)). If instead you want to have the species densities and the electron temperature time-averaged, then you must call the `define_bulk_solver` command with `time_average_solution=true` and pass the name of the bulk solver to the `solve_reactor` command (see [solve_reactor on page 548](#)).

Sheath Simulation With Pulsed Power and Multiple Bias Sources

The species density waveforms and the electron temperature waveform computed by the bulk model serve as input for the sheath model. Internally, the sheath solver needs to find the least common multiple of the periods of the different input waveforms (densities and electron temperature from the bulk model) and of the bias sources applied to the sheath. You can control the tolerance used to find the common period by using the parameter `frequency_snapping_period` in the `define_sheath_solver` command (see

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[define_sheath_solver on page 330](#)). In addition, you can increase the maximum number of periods considered by using the parameter `max_num_waveform_periods`.

When passing time-dependent density and electron temperature waveforms to the sheath model, the solution of the sheath model (the flux) is a time-dependent waveform as well. By default, however, the flux waveform is returned as time averaged and can be used to define a (time-independent) flux distribution for a PMC simulation (see [define_species_distribution on page 337](#)). If instead you want to work with a time-dependent flux waveform, then you must set `time_average_solution=false` in the `define_sheath_solver` command and pass the name of the sheath solver to the `solve_reactor` command (see [solve_reactor on page 548](#)).

Note:

The distribution of energies and angles of the flux is always averaged over one period of the flux waveform. Only the total flux (that is, the integral of the energy- and angle-dependent distribution) is time dependent.

If you pass a time-dependent flux distribution to the PMC simulator, then you can optionally specify the sampling time step used for the flux distribution in the PMC simulator:

```
define_species_distribution name=<c> type=plasma species=<c>
(solution=<c> | solution_file=<c>) [sampling_time_step=<n>]
```

You can visualize the time-dependent flux by saving the parameters of the species distribution to a TDR file (see [save on page 521](#)):

```
save species_distribution=<c> output_type=parameters time=<n>
```

Plasma Sheath Models

While the plasma bulk region is assumed to be spatially uniform, charge neutral, and homogeneous, there exists a region with a high electrical potential drop between the plasma bulk and the electrode: the so-called plasma sheath region.

In this region, ions accelerate strongly from the plasma bulk region towards the wafer surface. For the modeling of industrial plasma etching processes, it is essential to know the energy and angular distribution of the particles reaching the wafer surface. While the distribution in the plasma bulk region is isotropic in the thermodynamic equilibrium, the distribution changes considerably due to the acceleration of ions across the sheath layer.

You select the sheath models by using the `sheath_model_type` parameter in the command `define_plasma_model` (see [define_plasma_model on page 298](#)).

The next sections present different sheath models that predict the energy and angular distributions of ions and neutrals at the surface. In addition, unless otherwise stated, input parameters refer to the `define_reactor` command (see [define_reactor on page 301](#)).

Self-Consistent Circuit RF Sheath Model

A self-consistent dynamic model of the RF-biased sheath has been proposed by Edelberg and Aydil [10]. You select this model by setting `sheath_model_type=circuit` in the command `define_plasma_model`.

The circuit RF sheath model consists of two modules, which are coupled self-consistently:

- The first module is an ion transport model, which describes the charge transport in the sheath by solving the ion continuity equation, the ion momentum equation, and the Poisson equation for the sheath potential.
- The second module is an equivalent circuit model, which describes the sheath by a parallel electrical circuit consisting of a diode, a current source, and a capacitor connected to the applied RF bias source [10].

In the model, it is assumed that the sheath is infinite in the directions parallel to the electrode surface, such that the system reduces to a one-dimensional problem in the z-direction orthogonal to the surface. The model is suitable for industrial plasma reactors, which typically operate at high bias frequencies (in the MHz range) and low pressures (in the mTorr range). This implies that particles crossing the sheath can be assumed to be collisionless, as their mean free path (several millimeters) is typically much larger than the thickness of the sheath (several hundred micrometers).

Based on the sheath thickness $d_s(t)$ computed by the sheath model, the equivalent circuit model predicts the time-dependent waveform of the sheath potential at the electrode $V_w(t)$, which serves as a boundary condition for the Poisson equation. From the solution of the Poisson equation, a new value for the sheath thickness $d_s(t)$ is obtained, and the procedure is repeated self-consistently until the wall potential $V_w(t)$ converges to a periodic steady-state waveform (see [Figure 21 on page 111](#)).

To further analyze the simulation results for the circuit sheath model, you can save and visualize various datasets such as the wall potential $V_w(t)$, the sheath thickness $d_s(t)$, the currents through the sheath (applied RF bias current, electron current, total ion current, and capacitive displacement current), the sheath capacitance, the electric field at the wall, the fluxes, and the energy distributions of the ions or neutrals passing the sheath. For details about the datasets, see also [10]. You can extract datasets of interest by calling the `define_extraction` command with the parameters `type=plasma` and `sheath_model_type=circuit` (see [define_extraction on page 252](#)).

After the sheath potential profile at the wall $V_w(t)$ has converged, the energy distribution of the ions crossing the sheath potential is computed from the wall potential [10].

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Plasma Sheath Models

As for the analytic sheath model, [Equation 72](#), the full ion energy and angular distribution (IEAD) for ion species i is computed from the ion energy distribution (IED) by:

$$\text{IEAD}_i(E, \theta, \phi) \propto \text{IED}_i(E) \cdot \frac{1}{\cos^2 \theta} \cdot \exp\left(-\frac{E}{T_i} \tan^2 \theta\right) \quad (55)$$

where:

- $\theta \in [0, \pi/2]$ is the polar angle.
- $\phi \in [0, 2\pi]$ is the azimuth angle.
- E is the ion energy in eV.
- T_i is the ion temperature in eV, which is assumed to equal the neutral gas temperature in the plasma bulk region (given by the `gas_temperature` parameter).

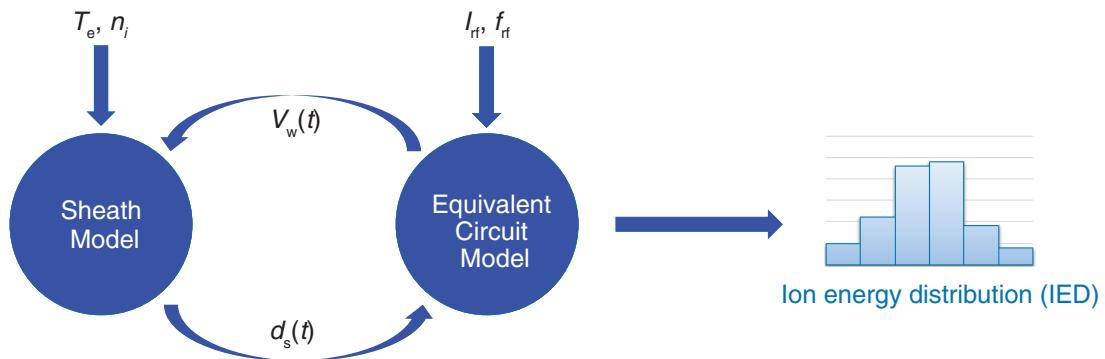
See [\[11\]](#) for details on the derivation of the ion angular distribution.

The IEAD satisfies the normalization condition:

$$\int_{E_{\min}}^{E_{\max}} dE \int_0^{2\pi} d\phi \int_0^{\pi/2} \sin \theta d\theta \text{IEAD}_i(E, \theta, \phi) = \Gamma_i \quad (56)$$

where Γ_i denotes the total flux of ion species i .

Figure 21 Flow chart of the model by Edelberg and Aydil used to predict the ion energy distribution (IED) of ions impinging on an RF-biased electrode, showing the self-consistent coupling between the sheath model and the equivalent circuit model. T_e and n_i denote the electron temperature and ion densities, I_{rf} and f_{rf} denote the RF bias current and frequency, and $V_w(t)$ and $d_s(t)$ denote the wall potential and sheath thickness, respectively.



Biasing Modes and Bias Pulsing

The model supports different biasing modes, which can be specified in the command `define_reactor` for a circuit sheath model (see [define_reactor on page 301](#)):

- [Current-Driven Mode](#)
- [Voltage-Driven Mode](#)
- [Power-Driven Mode](#)

Current-Driven Mode

In this mode, you can set the RF bias current $I(t)$ through the sheath as input to the sheath model. The resulting RF bias voltage $V_w(t)$ (wall potential) at the electrode is computed self-consistently to satisfy the current balance equation [10].

CDM1 Apply a sinusoidal RF bias current:

$$I(t) = I_{rf} \cdot \sin(2\pi f_{rf} t) \quad (57)$$

where I_{rf} is the amplitude of the bias current (parameter `rf_bias_current`), and f_{rf} is the bias frequency (parameter `rf_bias_frequency`).

CDM2 Apply multiple RF bias current sources with multiple frequencies:

$$I(t) = I_1(t) + I_2(t) + \dots = I_1 \cdot \sin(2\pi f_1 t) + I_2 \cdot \sin(2\pi f_2 t) + \dots \quad (58)$$

where $\{I_i\}$ are the amplitudes and $\{f_i\}$ are the frequencies. You can set these parameters by passing a list of values to the parameters `rf_bias_current` and `rf_bias_frequency`, respectively.

CDM3 Define an arbitrary time-dependent function expression for the RF bias current:

$$I(t) = f(t) \quad (59)$$

where the function $f(t)$ must be specified as a string in the `bias_current_waveform` parameter. (For information about the syntax for function expressions, see [Syntax for Expressions on page 139](#).) The bias current waveform is assumed to be periodic in time with a period given by parameter `bias_current_period`. By default, the bias current function is sampled using 100 points per period, which can be changed by using the parameter `num_waveform_samples`.

Voltage-Driven Mode

In this mode, you can set the RF voltage $V_w(t)$ (wall potential) applied to the electrode as input to the sheath model. The resulting RF bias current $I(t)$ through the sheath is computed self-consistently to satisfy the current balance equation [10].

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Plasma Sheath Models

VDM1 Apply a sinusoidal RF bias voltage:

$$V_w(t) = V_{DC} + V_{AC} \cdot \sin(2\pi f_{rf} t) \quad (60)$$

where V_{DC} and V_{AC} are the DC part and AC part of the wall potential, respectively, and f_{rf} is the bias frequency. You can only set V_{AC} and f_{rf} (parameters `rf_bias_voltage` and `rf_bias_frequency`) since the DC part is computed self-consistently to satisfy the current balance equation (for details, see [12]).

VDM2 Apply multiple RF bias voltage sources with multiple frequencies:

$$\begin{aligned} V_w(t) &= V_{DC} + V_1(t) + V_2(t) + \dots \\ &= V_{DC} + V_1 \cdot \sin(2\pi f_1 t) + V_2 \cdot \sin(2\pi f_2 t) + \dots \end{aligned} \quad (61)$$

where V_{DC} is the DC part of the sheath potential, $\{V_i\}$ are the AC amplitudes per frequency and $\{f_i\}$ are the frequencies. You can set parameters $\{V_i\}$ and $\{f_i\}$ by simply passing a list of values to parameters `rf_bias_voltage` and `rf_bias_frequency`, respectively. V_{DC} is determined self-consistently following [12].

VDM3 Define an arbitrary time-dependent function expression for the RF bias voltage:

$$V_w(t) = f(t) \quad (62)$$

where the function $f(t)$ must be specified as a string in the `wall_potential_waveform` parameter. (For information about the syntax for function expressions, see [Syntax for Expressions on page 139](#).) The bias voltage waveform is assumed to be periodic in time with a period given by parameter `wall_potential_period`. By default, the wall potential function is sampled using 100 points per period, which can be changed by the `num_waveform_samples` parameter.

Power-Driven Mode

In this mode, you can set the RF bias power P_{rf} applied to the electrode as input to the sheath model. The power-driven mode is a special case of the other biasing modes: instead of specifying the current or voltage explicitly, you set the power absorbed by the system. This implicitly determines the RF bias current $I(t)$ and the wall potential $V_w(t)$ through the relation:

$$P_{rf} = -\frac{1}{\tau} \int_0^\tau V_w(t) \cdot I(t) \, dt \quad (63)$$

where $\tau = 1/f_{rf}$ is the period of the wall potential $V_w(t)$ and of the bias current $I(t)$.

PDM1 Specify the RF bias power for a sinusoidal RF bias current (see **CDM1**):

$$P_{rf} = -\frac{1}{\tau} \int_0^\tau V_w(t) \cdot I_{rf} \sin(2\pi f_{rf} t) \, dt \quad (64)$$

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You must set `bias_mode=current_driven` and specify the power P_{rf} (parameter `rf_bias_power`) and the frequency (parameter `rf_bias_frequency`). The current amplitude I_{rf} and the wall potential waveform $V_w(t)$ are computed self-consistently to match the given RF bias power P_{rf} .

PDM2 Specify the RF bias power for a sinusoidal RF bias voltage (see **VDM1**):

$$P_{\text{rf}} = -\frac{1}{\tau_{\text{rf}}} \int_0^{\tau_{\text{rf}}} (V_{\text{DC}} + V_{\text{AC}} \cdot \sin(2\pi f_{\text{rf}} t)) \cdot I(t) \, dt \quad (65)$$

You must set `bias_mode=voltage_driven` and specify the power P_{rf} (parameter `rf_bias_power`) and the frequency (parameter `rf_bias_frequency`). The voltages V_{DC} and V_{AC} and the current waveform $I(t)$ are computed self-consistently to match the given RF bias power P_{rf} .

PDM3 Specify the RF bias power for multiple RF bias current sources (see **CDM2**):

$$P_{\text{rf}} = -\frac{1}{\tau} \int_0^{\tau} V_w(t) \cdot (I_1 \cdot \sin(2\pi f_1 t) + I_2 \cdot \sin(2\pi f_2 t) + \dots) \, dt \quad (66)$$

You must set `bias_mode=current_driven` and provide a list of frequencies $\{f_i\}$ (parameter `rf_bias_frequency`) and a list of power values per frequency $\{P_i\}$ (parameter `rf_bias_power`), where the power per frequency is defined by:

$$P_i = -\frac{1}{\tau} \int_0^{\tau} V_w(t) \cdot I_i \sin(2\pi f_i t) \, dt \quad (67)$$

As in **PDM1**, the current amplitudes $\{I_i\}$ and the wall potential waveform $V_w(t)$ are computed self-consistently to match the given powers per frequency $\{P_i\}$.

PDM4 Specify the RF bias power for multiple RF bias voltage sources (see **VDM2**):

$$P_{\text{rf}} = -\frac{1}{\tau} \int_0^{\tau} (V_{\text{DC}} + V_1 \cdot \sin(2\pi f_1 t) + V_2 \cdot \sin(2\pi f_2 t) + \dots) \cdot I(t) \, dt \quad (68)$$

You must set `bias_mode=voltage_driven` and provide a list of frequencies $\{f_i\}$ (parameter `rf_bias_frequency`) and a list of power values per frequency $\{P_i\}$ (parameter `rf_bias_power`), defined by:

$$P_i = -\frac{1}{\tau} \int_0^{\tau} V_i \cdot \sin(2\pi f_i t) \cdot I(t) \, dt \quad (69)$$

Analogously to **PDM3**, the voltages V_{DC} and $\{V_i\}$ and the current waveform $I(t)$ are computed self-consistently to match the given powers per frequency $\{P_i\}$.

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Note:

In the power-driven mode, the voltage and current waveforms are computed self-consistently by an iterative scheme. You can control the initial values of the iterative scheme by specifying the parameter `initial_rf_current` or `initial_wall_potential` in the `define_sheath_solver` command for `sheath_model_type=circuit` (see [define_sheath_solver on page 330](#)).

To monitor the convergence towards the target bias power, you can save and visualize the solution variables ($\{I_i\}$ or $\{V_i\}$) and the target powers (P_{rf} and $\{P_i\}$) as a function of the iteration number (see `define_extraction` with quantities `rf_bias_power_iterations`, `rf_bias_current_iterations`, or `rf_bias_voltage_iterations`).

To monitor the convergence errors as a function of the iteration, specify the quantities `rf_bias_power_residuals` and `wall_potential_residuals`.

If there are convergence issues, then you can decrease the values of parameter `power_relaxation_constant`, `max_rf_current_step`, or `max_rf_voltage_step` in the `define_sheath_solver` command. By changing the value of `power_tolerance`, you can influence when the iterative scheme is considered to have converged to the target power value.

Analytic RF Sheath Model

Another RF sheath model is the analytic model by Benoit-Cattin and Bernard [13]. You select it by setting `sheath_model_type=analytic` in the `define_plasma_model` command (see [define_plasma_model on page 298](#)).

The analytic RF sheath model predicts a bimodal ion energy distribution (IED) with two symmetric energy peaks, which are separated by a certain energy width ΔE . It is assumed that the sheath is one-dimensional in the z-direction orthogonal to the surface, and that the plasma reactor is operated at high bias frequencies (in the MHz range) and low pressures (in the mTorr range), such that collisions between particles in the sheath can be neglected.

The RF-modulated electric potential between the sheath edge at the plasma bulk boundary and the electrode on the wafer surface is described by:

$$V(t) = V_{DC} + V_{AC} \sin(2\pi f_{rf} t) \quad (70)$$

where:

- V_{DC} is the DC part of the sheath potential (specified by the `dc_voltage` parameter).
- V_{AC} is the AC part of the sheath potential (specified by the `ac_voltage` parameter).
- f_{rf} is the RF bias frequency (specified by the `rf_bias_frequency` parameter).

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Plasma Sheath Models

With the given sheath potential, the IED of ion i is computed to be [13][14]:

$$\text{IED}_i(E) \propto \frac{1}{\sqrt{1 - \frac{4(E - V_{\text{DC}})^2}{\Delta E_i^2}}} \quad (71)$$

where E denotes the ion energy in eV, and ΔE_i is the width of the IED in eV.

Given the IED, the full energy and angular distribution (IEAD) of ion species i reads:

$$\text{IEAD}_i(E, \theta, \phi) \propto \text{IED}_i(E) \cdot \frac{1}{\cos^2 \theta} \cdot \exp\left(-\frac{E}{T_i} \tan^2 \theta\right) \quad (72)$$

where:

- $\theta \in [0, \pi/2]$ is the polar angle.
- $\phi \in [0, 2\pi]$ is the azimuth angle.
- E is the ion energy in eV.
- T_i is the ion temperature in eV, which is assumed to equal the neutral gas temperature in the plasma bulk (given by the `gas_temperature` parameter).

See [11] for details on the derivation of the ion angular distribution.

The IEAD satisfies the normalization condition:

$$\int_{E_{\min}}^{E_{\max}} dE \int_0^{2\pi} d\phi \int_0^{\pi/2} \sin \theta d\theta \text{IEAD}_i(E, \theta, \phi) = \Gamma_i \quad (73)$$

where Γ_i denotes the total flux of ion species i .

For capacitively coupled plasma discharges (`reactor_type=ccp`), instead of specifying the sheath potential itself, you can define the RF voltage, $V_{\text{rf}} \sin(2\pi f_{\text{rf}} t)$, applied between the two parallel plates of the discharge. According to [6], the AC and DC sheath potentials are related to the applied RF voltage by:

$$V_{\text{DC}} = \frac{V_{\text{AC}}}{2} \approx 0.83 \frac{V_{\text{rf}}}{2} \quad (74)$$

The applied RF voltage can be specified by the following input parameters:

- `rf_bias_frequency` defines the RF bias frequency.
- `rf_voltage` defines the amplitude of the RF voltage waveform.

Sheath Model for Neutral Species

Both the circuit sheath model (`sheath_model_type=circuit`) and the analytic sheath model (`sheath_model_type=analytic`) treat neutral species in the same way.

Neutral plasma particles are not affected by the sheath potential, which implies that their energy and angular distribution at the electrode, after crossing the sheath, is the same as in the plasma bulk region. It is assumed that the energy distribution (ED) of neutral species n in the plasma bulk region is given by a Maxwell–Boltzmann distribution:

$$\text{ED}_n(E) = \frac{2\Gamma_n}{T_n^{3/2}\sqrt{\pi}} \exp\left(-\frac{E}{T_n}\right) \quad (75)$$

where:

- E is the energy in eV.
- $\Gamma_n = n_n v_n$ is the total flux of neutral n , where:
 - n_n is the plasma bulk density of neutral n .
 - $v_n = \sqrt{8eT_n/\pi m_n}$ is the thermal velocity of neutral n , where m_n is the mass of neutral n (specified in the `add_species` command; see [add_species on page 205](#)).
- T_n is the temperature of neutral n in eV (given by the `gas_temperature` parameter of the `define_reactor` command; see [define_reactor on page 301](#)).

Assuming an isotropic angular distribution, the full energy and angular distribution (EAD) of neutral species n reads:

$$\text{EAD}_n(E, \theta, \phi) \propto \text{ED}_n(E) \cdot \cos\theta \quad (76)$$

where $\theta \in [0, \pi/2]$ is the polar angle. The EAD satisfies the normalization condition:

$$\int_{E_{\min}}^{E_{\max}} dE \int_0^{2\pi} d\phi \int_0^{\pi/2} \sin\theta d\theta \text{EAD}_n(E, \theta, \phi) = \Gamma_n \quad (77)$$

Possible Issues and Recommendations

This section presents recommendations and possible issues that might be encountered when working with plasma models.

General Recommendations

The following are general recommendations:

1. Check that the plasma model operates in a suitable parameter range, as follows:
 - `ac_voltage` ∈ [10 V, 500 V]
 - `dc_voltage` ∈ [10 V, 500 V]
 - `densities` ∈ [10¹⁴ m⁻³, 10²¹ m⁻³]

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- electron_temperature ∈ [1 eV, 10 eV]
 - gas_temperature ∈ [200 K, 400 K]
 - inlet_gas_flow ∈ [1 sccm, 100 sccm]
 - power ∈ [100 W, 2500 W]
 - pressure ∈ [10⁻² mTorr, 100 mTorr]
 - rf_bias_current ∈ [1 A, 50 A]
 - rf_bias_frequency ∈ [0.1 MHz, 100 MHz]
 - rf_bias_power ∈ [1 W, 200 W]
 - rf_voltage ∈ [10 V, 500 V]
2. Check whether all parameters are specified in the correct physical units. Reaction rate coefficients (a, b, c, d, e, and energy_threshold) can be specified for the electron temperature in eV or K.

Common Mistakes

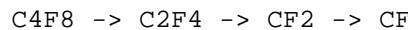
The following are common mistakes that can occur when setting up plasma models:

- rf_bias_frequency=3e6<MHz> instead of rf_bias_frequency=3<MHz>
- mass=6e-26 instead of mass=40 (default unit: <amu>)
- pressure=10 instead of pressure=10<mTorr> (default unit: <Pa>)
- gas_temperature=30 instead of gas_temperature=303.15 (default unit: <K>)

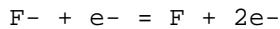
Reaction Data

The plasma bulk reaction datasets must be consistent and sufficiently complete to recover meaningful physical results. This means:

- Every reactant species should have been produced by another process. It must be a product of another reaction, or it must be specified as an inlet gas species (inlet_gas_flow parameter).
- For every meta-stable reaction byproduct, there should be another reaction that transforms the byproduct into a more stable product. For example:
 - Molecules in excited states, for example: Ar*
 - Nonatomic molecules, which can further split up, for example:



- For every negatively charged reaction product, there should be another reaction that transforms the negative ion into a neutral species. For example:



In addition, a common source of error is incorrect reaction rate coefficients. Incorrect numbers, signs, or physical units in reaction rate coefficients (parameters `a`, `b`, `c`, `d`, `e`, and `energy_threshold`), even if occurring only in a single reaction, can significantly change the result or lead to an overall failure of the model (typically in a negative density or negative electron temperature).

Negative Electron Temperature or Negative Species Density

You might encounter a negative electron temperature or negative species density during the bulk simulation. This error occurs in the plasma bulk model.

Possible solutions are:

- Use different initial conditions for the species densities (parameter `density` in the `define_reactor` command) or for the electron temperature (`electron_temperature` parameter).

Recommendations:

- Initialize most neutral or negatively charged species with zero density.
- The density n_i of the inlet gases (parameter `inlet_gas_flow`) must correspond to the given pressure p (parameter `pressure`) and gas temperature T_{gas} (`gas_temperature` parameter), that is:

$$\sum_{i \in \text{inlet gases}} n_i = \frac{p}{k_B T_{\text{gas}}}$$

- Do not specify the densities of the positive ions. Let the model chose them automatically.
- Configure the numeric parameters of the bulk solver, using [define_bulk_solver on page 210](#).

Recommendations:

- When simulating pulsed powers, decrease `pressure_relaxation_time` or `min_density_relaxation_time` to prevent undershooting toward negative values. You can also increase the cutoff parameters `min_density`, `min_electron_density`, or `min_electron_energy_density`.
- Decrease the initial step size of the solver (parameter `step_size`).

- Decrease the stepper errors (parameters `abs_error` and `rel_error`).
 - Vary the `stationary_state_tolerance` parameter.
3. See also [Reaction Data on page 118](#).

Convergence of Bulk Model

If your plasma bulk model takes a long time to converge, consider the following:

- Monitor the progress of the bulk simulation by writing out the bulk state and the convergence residuals (quantities `state` and `residuals` in [define_extraction on page 252](#)) at regular file update steps (parameter `file_update_step`). By monitoring the bulk state, you can check whether the solver proceeds.
- When using pulsed powers, initialize the reactor state with the steady-state solution of an equivalent continuous-wave power simulation, using the time-average value of the power waveform (parameter `solution` or `solution_file` in [define_reactor on page 301](#)).
- Increase the threshold for convergence, parameter `stationary_state_tolerance` in the `define_bulk_solver` command, to see whether the system converges at all.

Note:

Increasing the convergence threshold can lead to nonphysical results.

- Change the interval at which convergence is checked (parameter `convergence_check_step`).
- Consider increasing the value of parameters `pressure_relaxation_time` and `min_density_relaxation_time` in [define_reactor on page 301](#).
- Slightly change the process conditions to see whether the system converges in a test simulation under different conditions. If yes, then you can use the steady-state solution of the test simulation as an initial state for the actual simulation. See parameter `solution` or `solution_file` in [define_reactor on page 301](#).

Convergence of Circuit Sheath Model

The circuit sheath model might not converge to the specified RF bias power or might not converge to a self-consistent solution.

If the progress is slow during the iterative scheme, then consider the following:

- Monitor the progress of the sheath simulation by writing out the RF bias power, current, or voltage as a function of the iteration (quantities `rf_bias_power_iterations`, `rf_bias_current_iterations`, or `rf_bias_voltage_iterations` in the

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Possible Issues and Recommendations

`define_extraction` command; see [define_extraction on page 252](#)). To monitor the convergence errors as a function of the iteration, use the quantities `rf_bias_power_residuals` and `wall_potential_residuals`.

- Increase the number of iterations, by using the `max_rf_bias_power_iterations`, `max_sheath_iterations`, `max_sheath_width_iterations`, and `max_wall_potential_iterations` parameters in the `define_sheath_solver` command.
- Optimize the relaxation toward the target bias power by using the `power_relaxation_constant`, `max_rf_current_step`, or `max_rf_voltage_step` parameter in the `define_sheath_solver` command.
- Increase the value of `power_tolerance` to increase the threshold for convergence toward the target bias power.
- Slightly change the initial values of the sheath model, by using the parameters `initial_rf_current`, `initial_sheath_width`, and `initial_wall_potential`.

If the sheath model stops with an error:

- In the simulation log file, analyze the densities of the positive ions computed by the bulk model. The sum of the densities of all positive ions should be in the range [10^{14} m^{-3} , 10^{18} m^{-3}]. If ion densities are too low, then increase the reactor parameter `power` or `pressure`. If ion densities are too high, then decrease `power` or `pressure`.
- If you use time-dependent waveforms for the densities and the electron temperature as input to the sheath model (resulting from a plasma bulk simulation with pulsed power), then you can instead use the time-averaged values by setting `time_average_solution=false` in the `define_bulk_solver` command of your bulk model.
- If you use a user-defined function expression for the bias source applied to the sheath (parameter `wall_potential_waveform` or `bias_current_waveform`), then you can increase the number of samples used to discretize the function by using the parameter `num_waveform_samples`.

If the progress is slow during computation of the energy- and angle-dependent flux distribution (EAD):

- Reduce the resolution of the EAD by decreasing `num_angle_samples`, `num_energy_samples`, and `num_inv_cdf_histogram_bins` in the `define_sheath_solver` command.
- If using the Monte Carlo IED solver (`ied_solver=monte_carlo`), then reduce the number of samples (parameter `num_monte_carlo_samples` in the `define_sheath_solver` command).

Energy or Angle Resolution of IEAD Is Too Coarse

The energy or angle resolution of the IEAD might be too coarse.

To resolve this, increase the values of the following parameters in the command `define_sheath_solver`:

- `num_angle_samples`
 - `num_energy_samples`
 - `num_ied_histogram_bins`
 - `num_inv_cdf_histogram_bins`
-

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5

Surface Charging

This chapter describes surface charging in PMC simulations.

Overview of Surface Charging

An important phenomenon commonly observed in high aspect ratio plasma etching is surface charging inside the feature [1]. During plasma etching, the surface is constantly exposed to charged particles from the plasma, such as ions and electrons, impinging on the surface. At the surface, some of the ions and electrons transfer their charge to the surface. If the surface is a dielectric, then the charges cannot flow away and build up in time. Every surface charge acts as a source of an electric field, which deflects the trajectories of subsequent ions and electrons entering the feature [1][2].

The consequences of surface charge-up are significant: common artifacts attributed to the charge-up effect are sporadic bending and twisting of holes and trenches in dielectrics, notching and microtrenching at the feature bottom, and even early etch stop [1][2][3] [4][5][6].

The charge-up feature in Sentaurus Topography 3D PMC aims to model the surface charging effect during feature etching and deposition processes. The model consists of different parts:

- Ion and electron transport through an electric field (see [Ion and Electron Transport Through an Electric Field on page 125](#))
- Transfer of impinging charges to the surface (see [Transfer of Impinging Charges to the Surface on page 126](#))
- Modeling electric material properties (dielectrics, conductors, and applied electric potentials) (see [Electric Material Properties on page 127](#))
- Computation of the electric field caused by surface charges and applied electric potentials (see [Electric Field Computation on page 128](#))

Ion and Electron Transport Through an Electric Field

This section explains ion and electron transport through an electric field.

Ion Properties and Flux Distribution

When moving through an electric field, charged particles encounter a Coulomb force influencing the trajectory of the moving charge [2]. Depending on the local strength and orientation of the electric field, flying charges can be accelerated or decelerated, deflected sideways, or even repelled back into the plasma [2][5]. The influence of the electric field on the trajectories of charged particles depends on the charge, mass, and velocity of the particles.

Therefore, to simulate charged particle sources, first an energy- and angle-dependent flux distribution ([define_species_distribution command](#); [define_species_distribution on page 337](#)) must be specified, from which the initial velocities and directions of the source particles are sampled. Second, the mass and charge of the flux species must be specified by calling the [define_species_properties command](#) (see [define_species_properties on page 355](#)):

```
define_species_properties name=<c> species=<c> mass=<n> charge=<n>
```

The mass must be entered in atomic mass units, and the charge in units of the unit charge.

Electron Flux Distribution

While the main surface-changing reactions such as sputtering, etching, and deposition are driven by heavy ions and neutral radicals, charge-up is strongly influenced by electrons [1][2][3]. The flux and species properties for electrons do not need to be defined explicitly. When using the PMC charge-up model, electrons are simulated by default with thermal energies of 1 eV and with an isotropic flux distribution, $f(\theta) = 1/\pi\Gamma_e \cos(\theta)$, where the total electron flux Γ_e is implicitly set equal to the total ion flux to satisfy the overall charge neutrality condition [1][3][7].

A user-defined electron flux distribution is input by providing a list of exponent parameters $\{m_i\}$ and flux values $\{\Gamma_i\}$ for a generalized electron angular distribution:

$$f(\theta) = \frac{1}{2\pi} \sum_i \Gamma_i \cdot (m_i + 1) \cdot \cos^{m_i}(\theta)$$

See the parameters `electron_exponents` and `electron_fluxes` in the `define_charging_model` command (see [define_charging_model on page 213](#)).

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Transfer of Impinging Charges to the Surface

In addition, for user-defined electron distributions, the total electron flux $\Gamma_e = \sum_i \Gamma_i$ is rescaled to match the total ion flux (charge neutrality condition). This rescaling can be switched off by setting `enforce_charge_neutrality=false` in the `define_charging_model` command.

Starting Position of Charged-Particle Trajectories

Since charged particles move through an electric field, the starting position of the charged particles can affect the simulation results. To change the vertical position of the plane from which the charged particles start, use parameter `source_position` in the `define_etch_machine` command (see [define_etch_machine on page 242](#)).

Note:

The source position must lie inside the simulation domain.

To extend the simulation domain in the vertical direction, you can add a layer of Gas by using the `fill material=Gas thickness=<n>` command or the parameter `top_gas_thickness` in the `etch` or `filter_structure` command.

Transfer of Impinging Charges to the Surface

At the surface, incoming ions and electrons transfer their charges to the surface. During an etching or deposition process, the surface charges move with the dynamically evolving surface. To control the amount of charges transferred to the surface, you can set the `charging_factor` parameter in the `define_charging_model` command (see [define_charging_model on page 213](#)).

By calibrating this parameter, you can effectively control the strength of the charge-up effect in your simulation. This allows you to calibrate the model to experimental data using a single `charging_factor` parameter. Reasonable values for the `charging_factor` lie in the order of 1. Alternatively, you can explicitly set the dose of charges deposited on the surface (parameter `charge_dose`), which gives you full control over the charge-up. The charge dose is defined as the number of charges per area of a flat reference surface.

To improve the statistics and smoothness of the results, you can optionally increase the number of samples sent to the surface during a charge-up simulation (parameter `num_samples_per_cell`). Internally, when increasing the number of samples, the charge per sample is reduced proportionally such that the physical total charge stays invariant. Equivalently, the charge per sample can be reduced (parameter `charge_scaling`), which will result in an up-scaling of the number of samples to keep the total charge fixed. (Charge scaling is simply a numeric optimization to smooth the distribution of charges along the surface. It affects neither the ion and electron trajectories nor the charge density used for the electric field computation.)

Electric Material Properties

For a realistic evaluation of the electric field induced by surface charges, it is essential to know the electric properties of the materials. On dielectric or insulating surfaces, incoming charges are trapped and remain at localized positions [1]. On conducting surfaces, on the other hand, deposited charges flow away and spread immediately over the entire conductor surface. Even if materials are not exposed to the surface, polarization and capacitance effects inside these materials can still influence the electric field in the gas phase due to the long-range nature of the electrostatic force. Therefore, the electric properties of each material in the structure must be defined, regardless of whether or not the material is exposed to the surface.

Different types of medium can be defined using the `define_species_properties` command:

- A dielectric medium (by specifying its relative permittivity):

```
define_species_properties name=<c> species=<c> permittivity=<n>
```

- A conductor (by specifying any nonzero conductivity):

```
define_species_properties name=<c> species=<c> conductivity=<n>
```

Note:

The PMC charge-up model supports only ideal conductors. Any material with a nonzero conductivity is treated as an ideal conductor, that is, the value of the conductivity is not relevant for the electric field computation.

By default, conducting materials are treated as floating materials, which means that their electric potential is not fixed, but depends on their environment. To model a conductor with a fixed potential (for example, a grounded or contacted conductor), a constant electric potential can optionally be applied; it remains constant during the entire simulation even if the conductor surface is hit by incoming charges. To fix the potential on a conducting material, a (virtual) point-like contact at any location in the inside of the conductor must be specified:

```
define_electric_contact name=<c> position=<v> potential=<n>
```

See [define_electric_contact on page 238](#). Then, the name of the contact must be passed to the `define_charging_model` command.

Note:

For both floating and contacted conductors, the potential inside the conductor is spatially constant (general property of an ideal conductor). If two conducting materials touch, then they are automatically treated as a single joined conductor with a common spatially constant potential. If two floating conductors merge, then their total charges are summed. If a floating conductor and a contacted conductor

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merge, then the floating conductor acquires the fixed potential of the contacted conductor. If two conductors with different fixed potentials merge, then an error message is generated, stating that an electric shortcut has been detected.

The domain boundaries can also behave like conductors, for example, if the bottom boundary with Dirichlet boundary conditions is grounded at a fixed potential of 0 V.

Electric Field Computation

The electric field caused by the surface charges is updated at regular time intervals for the entire simulation domain. The update times can be set by the parameter `electric_field_update_interval` in the `etch` command (see [etch on page 399](#)).

At every electric field update, the main PMC simulation stops, and the new electric field is computed. The computation of the electric field requires solving the Poisson equation for the given charge distribution, inhomogeneous material properties, and boundary conditions (BC). This is performed by the electric field solver module called GRC.

Boundary Conditions

The BC for the electric field must be specified on all boundary planes of the simulation domain:

- On the lateral boundary planes at $x = x_{\min}$, $x = x_{\max}$, $y = y_{\min}$, and $y = y_{\max}$, the BC are adopted automatically from the specified structure (see [define_boundary_conditions on page 207](#)).

In the case of reflective BC, Neumann BC are used for the electric field, $\vec{E} \cdot \hat{n} = 0$, where \hat{n} denotes the surface normal of the boundary plane. In the case of periodic BC, the electric field also satisfies periodic BC:

$$\vec{E}(x_{\min}, y, z) = \vec{E}(x_{\max}, y, z), \vec{E}(x, y_{\min}, z) = \vec{E}(x, y_{\max}, z)$$

- On the bottom and top boundary planes at $z = z_{\min}$ and $z = z_{\max}$, three types of BC can be specified by using the parameters `bottom_bc` and `top_bc` in the `define_charging_model` command:

- `dirichlet`: Sets the electric potential ϕ on that boundary plane to a spatially constant value. The boundary potential value is set with the parameters `bottom_potential` and `top_potential` (default: 0 V).
- `neumann`: Sets the normal component of the electric field, $\vec{E} \cdot \hat{n}$, to a fixed value. By default, $\vec{E} \cdot \hat{n} = 0$ V/m, but the right-hand side value can be changed with the parameters `bottom_electric_field` and `top_electric_field`.

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Electric Field Computation

- floating: The value of the spatially constant potential is not fixed on the boundary plane, but computed by the solver. This BC allows you to model a floating conducting plane.

The BC at the bottom and top of the simulation domain can be chosen independently of each other, but you must set the value of the electric potential in at least one point to obtain a unique solution of the Poisson equation. A common practice is to use Dirichlet BC with $\phi=0$ V on the bottom plane and Neumann BC with $\vec{E} \cdot \hat{e}_z = E_z$ on the top plane, where E_z is the vertical component of the time-averaged electric field in the plasma sheath.

E_z can be either extracted from a plasma sheath simulation (see plasma extraction quantity `wall_electric_field_z`; see [Table 37](#)) or approximated by:

$$E_z = -\frac{|V_{DC}|}{d_s}$$

where V_{DC} is the DC part of the sheath potential, and d_s is the sheath thickness. Assuming typical values $V_{DC} = 100\text{--}1000$ V and $d_s = 1\text{--}10$ mm, the electric field E_z lies in the range from 10^4 to 10^6 V/m.

Poisson Solver: Guidelines

This section provides guidelines for working with the Poisson solver.

Choosing the Mesh Size of the Solver

Different optional parameters can be adjusted in the `define_electric_solver` command to optimize the speed, robustness, and accuracy of the Poisson solver. The most important parameter is `grc_grid_refinement_ratio`, which controls the mesh size of the Poisson solver in units of the PMC spacing.

For large domain sizes, to reduce computation time, you should successively increase the grid refinement ratio (preferably in powers of 2) until a reasonable balance between speed and accuracy is found. This might require carefully checking the consistency of the simulation results.

Optimizing the Solver Speed

Different solvers and preconditioning methods are available and can be selected by using the parameters `grc_solver` and `grc_preconditioner`. Depending on the problem, simulation speed is optimized by choosing a different solver or preconditioner or both.

The internal convergence thresholds of the iterative linear solver (parameters `grc_solver_abs_error` and `grc_solver_rel_error`) can also be configured for optimization. The absolute error is defined as the residuum of the linear equation system. If

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the absolute residuum becomes smaller than `grc_solver_abs_error`, then the solver is considered to have converged and the solution is returned. Otherwise, the relative error is computed, which is defined as the residual of the current iteration divided by the residual of the initial linear equation system. If the relative error becomes smaller than `grc_solver_rel_error`, then the solver is considered to have converged.

Note:

By default, `grc_solver_abs_error=0`, that is, the absolute error check is switched off. This is a reasonable starting point for solver optimization. To speed up convergence, you can increase `grc_solver_abs_error` slightly, while carefully checking the consistency of the simulation results.

Error Handling

Depending on the problem, the linear solver might fail to find a solution. In that case, by default, the computation restarts automatically with different solver and preconditioner settings (the automatic solver switch can be deactivated by using `grc_optimize_solver=false`).

The maximum number of solver iterations (`grc_max_num_iterations`) can be configured. If the number of iterations exceeds the maximum number of iterations, then an error message is generated. In that case, increase `grc_max_num_iterations`.

Choosing the Update Interval for the Electric Field

When simulating charge-up during a PMC etching or deposition simulation, a critical issue is how to choose the time interval at which the electric field is recomputed (parameter `electric_field_update_interval` in the `etch` command; see [etch on page 399](#)).

Theoretically, in an etching process or a deposition process, the electric field changes after every geometric change of the surface, which is after every executed PMC surface reaction. Practically, a reasonable balance needs to be found between accuracy and speed. A reasonable choice for the update time interval is the time span needed to etch or deposit a layer of one PMC spacing. An estimate for this time span can be obtained, for example, from the measured etching rate in a test simulation without charging.

To speed up the electric field update, it is reasonable to recompute the electric field only if the distribution of surface charges has changed significantly. Therefore, as an optimization, a threshold for the change of the surface charges (parameter `electric_field_update_accuracy` in the `etch` command) can optionally be set. If the change of the surface charges is less than `electric_field_update_accuracy`, then the electric field is not recomputed. The criterion for an electric field update is defined by:

$$\left(\int_{\Omega} (\rho(\vec{r}, t) - \rho(\vec{r}, t - \Delta t))^2 d^3 r \right)^{1/2} > \varepsilon \cdot \left(\int_{\Omega} \rho^2(\vec{r}, t) d^3 r \right)^{1/2} \quad (78)$$

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Plotting Electric Field, Potential, Charge Density, and Ion Trajectories

where $\rho(\vec{r}, t)$ denotes the charge density at time t , Δt is the electric field update interval, ε is the electric field update accuracy, and the integration is over the entire simulation domain Ω .

Plotting Electric Field, Potential, Charge Density, and Ion Trajectories

You can save datasets either at the end of a PMC simulation or during a PMC simulation (as intermediate plots at regular time intervals).

Available datasets are the electric field (vector field), the electric potential (scalar field), the charge density (scalar field), and the ion trajectories (1D lines).

Writing Charging Datasets at the End of a Simulation

To save a dataset at the end of a simulation, call the command:

```
save type=<c> [point_min=<v>] [point_max=<v>] [file=<c>]
```

where `type` is any of `electric_field`, `electric_potential`, or `charge_density`. For large domain sizes, the loading time of saved TDR files decreases by restricting the domain to the volume of interest using the parameters `point_min` and `point_max`.

Caution:

Ion trajectories cannot be plotted in the `save` command. To plot trajectories, use intermediate plots.

Writing Charging Datasets at Intermediate Time Points

To save intermediate plots while the simulation is running, call the `etch` command with the following parameters:

```
etch ... plot_type=<l> plot_interval=<n>
```

where `plot_type` is a list of datasets, for example, `electric_field`, `electric_potential`, `charge_density`, and `trajectories`. Note that, for charge-up-related datasets, the `plot_interval` must be a multiple of the `electric_field_update_interval`.

As an alternative to a regular plot interval, you can define a list of plot time points by using the parameter `plot_times`:

```
etch ... plot_type=<l> plot_times=<v> [plot_times_unit=<c>]
```

Chapter 5: Surface Charging

Plotting Electric Field, Potential, Charge Density, and Ion Trajectories

Analogously to `plot_interval`, each time point in `plot_times` must be a multiple of the `electric_field_update_interval`. To change the unit of the plot times, use the parameter `plot_times_unit`.

Before updating the file, you can use the parameter `plot_file_update_interval` to accumulate several plots. A common practice to avoid large output files is to write each intermediate plot to a separate file – one file for each time point – by setting `split_plots=true`.

Similar to the `save` command, the domain of the intermediate plots can be restricted to a sub-volume by using the parameters `point_min` and `point_max`.

Plotting Ion Trajectories

For charge-up simulations, it can be instructive to plot the trajectories of charged ions on their way from the plasma sheath toward the structure through the electric field. To plot the trajectories, add `trajectories` to the list of plot types in the `etch` command, or define an extraction with `type=trajectories` in the `define_extraction` command (see [etch on page 399](#) and [define_extraction on page 252](#)).

By default, 50 ion trajectories are plotted with random starting positions along the PMC source plane. If more than one ion flux is defined, then the species type of each trajectory is sampled according to the flux ratio of the ions.

To change the number of trajectories, use the parameter `num_trajectories` of the `etch` or `define_extraction` command. Alternatively, the precise starting positions of the ion trajectories on the source plane can be defined as a list of xy pairs in the parameter `trajectory_starting_positions`.

When using the command `define_extraction type=trajectories`, you can further specify the ion or neutral species, an energy window, and an end point volume (see [define_extraction on page 252](#)).

When loading the trajectory plots in Sentaurus Visual, the trajectories can be colorized to see the local ion velocity, kinetic energy, or charge along each trajectory.

Note:

The plotted trajectories are computed only for visualization purposes and are not connected to the actual PMC simulation. In particular, the parameters `num_trajectories` and `trajectory_starting_positions` have no influence on the actual PMC simulation.

Chapter 5: Surface Charging

Extracting the Electric Field, Potential, and Charge Density

Restarting the Simulation

To restart a charge-up simulation from the final state of a previous simulation, you can use a PMC file to transfer the structure and charge-up state from one simulation step to the next. Add `save type=pmc file=...` to the end of the simulation to save the structure and the charge-up state to the file.

To reload the structure and charge-up state, use `define_structure pmc_file=...` (see [define_structure on page 360](#)).

Extracting the Electric Field, Potential, and Charge Density

Different quantities can be extracted as a function of time, such as:

- Charge density for each bulk species in units of [e/nm³]
- Net charge density of all species in units of [e/nm³]
- Electric field (x-, y-, z-components, and the absolute value) in units of [V/m]
- Electric potential in units of [V]

All these quantities can be extracted in different formats:

- Scalar results (summed or averaged over a specified volume)
- Two-dimensional results (on an axis-aligned plane)
- Three-dimensional results (on a 3D bounding box)

The results are written to a TDR file, CSV file, or Tcl variable.

To define the extraction type, call the `define_extraction` command with `type=pmc_data` and provide a list of datasets (`charge_density`, `electric_field`, or `electric_potential`) in the parameter `quantities` (see [define_extraction on page 252](#)):

```
define_extraction name=<c> type=pmc_data quantities=<l>
```

The `define_extraction` command supports many other optional parameters:

- When extracting `charge_density`, you can specify a list of species names for which you want to extract the charge density (parameter `species`). By default, the charge density of **all** species is extracted.
- For large domain sizes, you can speed up the loading of saved TDR files by restricting the extraction domain to a sub-volume, using the parameters `point_min` and `point_max`.

Chapter 5: Surface Charging

Example Project

- By default, the mean value of each quantity is extracted as a function of time, averaged over the entire simulation domain (or, if specified, over the sub-volume defined by `point_min` and `point_max`). Alternatively, the maximum or minimum value, standard deviation, and sum or mean of the absolute values (parameter `operator=integral|mean|sum|max|min|stddev|sumabs|meanabs`) can be computed.
- Three-dimensional grid output can be produced for all quantities by setting `grid_output=true`.
- The quantities on a 2D cutplane, specified by a normal vector (parameter `axis`), and a point on the plane (parameter `position`) can be extracted.
- The extraction results can be saved in a Tcl variable by using the parameter `tcl_output_variable`.
- In addition to a TDR file, you can save the extraction results to a CSV file by specifying the parameter `csv_file`.
- The default grouping of the time-dependent datasets stored in a TDR file, which will affect the dataset grouping in Sentaurus Visual, can be changed. By default, datasets are labeled by a `pmc_data` tag. When setting `tdr_file_dataset_grouping=quantity`, datasets will be instead labeled by the quantity name in Sentaurus Visual.

Finally, you must register the name of the defined extraction in the `etch` command and specify a regular time interval at which the data is extracted:

```
etch ... extraction=<c> extraction_interval=<n>
```

In analogy to intermediate plots, a list of extraction time points can be provided instead:

```
etch ... extraction=<c> extraction_times=<v> [extraction_times_unit=<c>]
```

In addition, several plots can be accumulated before updating the file by using the parameter `extraction_file_update_interval`.

Note:

As for intermediate plots, the extraction time points must be a multiple of the `electric_field_update_interval`.

Example Project

The following code shows the essential parts of a command file for a charge-up simulation:

1. Flux distribution: Specify the energy distribution of ion fluxes. For realistic energy distributions, use the plasma model.

```
define_species_distribution name=sd species=I flux=1e-4 \
angle_spread=0.5 energy_min=10 energy_max=100
```

Chapter 5: Surface Charging

References

2. Species properties: For ion fluxes, mass and charge must be specified. For insulating materials, specify the permittivity. For conductors, specify a conductivity > 0. The exact value is not important.

```
define_species_properties name=sp species=I mass=40 charge=1
define_species_properties name=sp species=Photoresist \
    permittivity=4.2
define_species_properties name=sp species=Aluminum conductivity=1
```

3. Charging model and electric solver: Use these commands to define properties of the charging model and of the electric field solver.

```
define_charging_model name=cm charging_factor=1 \
    bottom_bc=dirichlet bottom_potential=0 \
    top_bc=neumann top_electric_field=-1e5

define_electric_solver name=es grc_grid_refinement_ratio=4
```

4. Etch machine: Add the charging model to the etch machine.

```
define_etch_machine model=mo species_distribution=sd \
    species_properties=sp charging_model=cm
```

5. Etch command: Specify the electric solver and the field update interval in the `etch` command.

```
etch spacing=0.001 time=1 method=pmc electric_solver=es \
    electric_field_update_interval=0.1
```

References

- [1] J. C. Arnold and H. H. Sawin, "Charging of pattern features during plasma etching," *Journal of Applied Physics*, vol. 70, no. 10, pp. 5314–5317, 1991.
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- [3] K. P. Giapis and G. S. Hwang, "Pattern-Dependent Charging and the Role of Electron Tunneling," *Japanese Journal of Applied Physics*, vol. 37, no. 4B, pp. 2281–2290, 1998.
- [4] M. A. Vyvoda, M. Li, and D. B. Graves, "Hardmask charging during Cl₂ plasma etching of silicon," *Journal of Vacuum Science & Technology A*, vol. 17, no. 6, pp. 3293–3307, 1999.
- [5] T. Kinoshita, M. Hane, and J. P. McVittie, "Notching as an example of charging in uniform high density plasmas," *Journal of Vacuum Science & Technology B*, vol. 14, no. 1, pp. 560–565, 1996.

Chapter 5: Surface Charging

References

- [6] J. Matsui *et al.*, "The effect of topographical local charging on the etching of deep-submicron structures in SiO₂ as a function of aspect ratio," *Applied Physics Letters*, vol. 78, no. 7, pp. 883–885, 2001.
- [7] M. Wang and M. J. Kushner, "High energy electron fluxes in dc-augmented capacitively coupled plasmas. II. Effects on twisting in high aspect ratio etching of dielectrics," *Journal of Applied Physics*, vol. 107, no. 2, p. 023309, 2010.

6

Input Commands

This chapter describes the Sentaurus Topography 3D input commands.

Command Syntax

All commands in Sentaurus Topography 3D follow the general structure:

```
command parameter1=value1 [parameter2=value2]
```

where `parameter1` and `parameter2` are parameters that are set to `value1` and `value2`, respectively.

Note:

Brackets denote optional parameters.

The type of parameter values is denoted by a character in angle brackets as follows:

- `` – Boolean (this is always either `true` or `false`)
- `<c>` – character string
- `<l>` – list of strings
- `<n>` – numeric value
- `<v>` – vector of numbers

Vectors are denoted using the Tcl array syntax (braces). For example, `{0 0 1}` is a vector normal to the horizontal plane.

- `<w>` – list of vectors of numbers

A vertical bar denotes exclusive options, such that either one parameter or another is expected by a command. For example:

```
command parameter1=value1 / parameter2=value2
```

Chapter 6: Input Commands

Command Syntax

Parentheses indicate grouping of parameters. Parentheses are *not* part of the syntax. For example:

```
[ (extraction_interval=<n> | \
    extraction_times=<v> [extraction_times_unit=<c>]) \
    [extraction_file_update_interval=<n>] \
    [force_intermediate_extraction=<b>]]
```

For examples, see [Appendix A on page 598](#).

Units

Sentaurus Topography 3D supports a set of default units (second column in [Table 7](#)) that is used whenever no unit is specified for a parameter in the command file.

You can use different units by specifying them in angle brackets after the numeric value. For example:

```
command parameter1=value1<unit1> [parameter2=value2<unit2>]
```

For example, the default unit for a rate is <um/min>. In the command file, you can also specify any of the measurement units listed in [Table 7](#) for velocity.

Table 7 Supported units in Sentaurus Topography 3D

Variable	Default		Other possible values	
	Unit	Symbol	Unit	Symbol
Angle	degree	<deg>	radian	<rad>
Angular velocity	revolution per minute	<rpm>	radian per second	<rad/s>
Density	gram per cubic centimeter	<g/cm ³ >	kilogram per cubic meter	<kg/m ³ >
Energy	electron volt	<eV>	joule	<J>
Length	micrometer	<um>	meter	<m>
			nanometer	<nm>
Surface tension	dyne per centimeter	<dyn/cm>	Newton per meter	<N/m>
Time	minute	<min>	second	<s>

Chapter 6: Input Commands

Command Syntax

Table 7 *Supported units in Sentaurus Topography 3D (Continued)*

Variable	Default		Other possible values	
	Unit	Symbol	Unit	Symbol
Velocity	micrometer per minute	<um/min>	meter per second	<m/s>
			micrometer per second	<um/s>
			nanometer per minute	<nm/min>
			nanometer per second	<nm/s>
Viscosity	poise	<poise>	Pascal second	<Pa*s>

Syntax for Expressions

Note:

Expressions are supported only if the GNU compiler gcc is installed on the system where Sentaurus Topography 3D is running and is globally available there.

The following expression types are supported:

- Time-dependent expressions
- Position-dependent expressions
- Angle-dependent expressions
- Energy-dependent expressions

Their syntax consists of the following components:

- Numeric constants containing the decimal point
- Arithmetic operators: +, -, *, /
- Mathematical constants:
 - `M_E` (denotes the value of the Euler number)
 - `M_PI` (denotes the value of π)
- Mathematical functions: `fabs(u)`, `sin(u)`, `cos(u)`, `tan(u)`, `asin(u)`, `acos(u)`, `atan(u)`, `atan2(v,u)`, `sinh(u)`, `cosh(u)`, `tanh(u)`, `exp(u)`, `log(u)`, `log10(u)`, `pow(u,v)`, `sqrt(u)`, `ceil(u)`, `floor(u)`, `fmod(u,v)`

The argument of the trigonometric functions must be given in radians.

Chapter 6: Input Commands

Command Syntax

- Relational functions:

```
high_pass(u, v, w), higher_pass(u, v, w)  
low_pass(u, v, w), lower_pass(u, v, w)
```

For definitions of these functions, see [Conditional and Relational Functions on page 573](#).

- `square_pulse(u, v_on, v_off, period, duty_cycle)`
 - `square_pulse` defines a square pulse function, that is, a periodic function with a `period` `period`. In the first part of each period, its value is `v_on`. In the second part of each period, its value is `v_off`. The length of the first part of the period is specified by the product of the duty cycle `duty_cycle` and the period `period`. `square_pulse` is defined such that a period starts when `u=0`.
 - `period` must have a positive value, and `duty_cycle` must belong to the [0,1] range.
- `square_pulse_arg_on(u, period)`
 - It returns the difference between `u` and the beginning of the period of a square pulse of period `period` to which `u` belongs.
 - `period` must have a positive value.
- `square_pulse_arg_off(u, period, duty_cycle)`
 - It returns the difference between `u` and the largest beginning of the second part of the period of a square pulse of period `period` and duty cycle `duty_cycle`, not larger than `u`.
 - `period` must have a positive value, and `duty_cycle` must belong to the [0,1] range.
- The conditional expression "condition ? u : v", returning `u` if `condition` is true, and `v` otherwise
- Parentheses
- For time-dependent and for position-dependent expressions:
 - `pwc(u, table)`
 - It returns the piecewise-constant interpolation of the values specified by `table` at value `u`.
 - The string `table` must have the following format:
$$(d_1, d_2, \dots, d_{2N-1}, d_{2N})$$
where `N` is an integer value greater than 1, and `d_n`, `n=1, \dots, 2N` is a numeric constant.

Chapter 6: Input Commands

Command Syntax

- The numeric constants specified by `table` represent the values to interpolate and must be such that $d_{2i-1} < d_{2i+1}$, for $i=1, \dots, N-1$.
- The numeric value returned by `pwc` is computed as follows:

$$pwc(u, (d_1, d_2, \dots, d_{2N-1}, d_{2N})) = \begin{cases} d_2 & \text{if } u \leq d_1 \\ d_2 & \text{if } d_1 \leq u < d_3 \\ d_4 & \text{if } d_3 \leq u < d_5 \\ \dots \\ d_{2N-2} & \text{if } d_{2N-3} \leq u < d_{2N-1} \\ d_{2N} & \text{if } u \geq d_{2N-1} \end{cases}$$

◦ `pwl(u, table)`

- It returns the piecewise-linear interpolation of the values specified by `table` at value `u`.
- The string `table` must have the following format:

$(d_1, d_2, \dots, d_{2N-1}, d_{2N})$

where `N` is an integer value greater than 1, and d_n , $n=1, \dots, 2N$ is a numeric constant.

- The numeric constants specified by `table` represent the values to interpolate and must be such that $d_{2i-1} < d_{2i+1}$, for $i=1, \dots, N-1$.

Chapter 6: Input Commands

Command Syntax

- The numeric value returned by `pwl` is computed as follows:

$$pwl(u, (d_1, d_2, \dots, d_{2N-1}, d_{2N})) = \begin{cases} d_2 & \text{if } u \leq d_1 \\ d_2 + \frac{d_4 - d_2}{d_3 - d_1}(u - d_1) & \text{if } d_1 \leq u < d_3 \\ d_4 + \frac{d_6 - d_4}{d_5 - d_3}(u - d_3) & \text{if } d_3 \leq u < d_5 \\ \dots \\ d_{2N-2} + \frac{d_{2N} - d_{2N-2}}{d_{2N-1} - d_{2N-3}}(u - d_{2N-3}) & \text{if } d_{2N-3} \leq u < d_{2N-1} \\ d_{2N} & \text{if } u \geq d_{2N-1} \end{cases}$$

- For time-dependent expressions:

- The string `t` denotes the numeric value of the current simulation time `t` in minutes.
- The string `t<unit>` denotes the numeric value of the current simulation time `t` in the specified unit (possible values for `<unit>` are `min` and `s`).
- `make_periodic(u, p, t)`
 - It returns a periodic function of `t` with period `p` minutes. The returned periodic function evaluates to the same values as `u` does for $0 \leq t < p$.
 - `p` is the numeric value of the period in minutes. It must be a nonnegative value.

Note:

If `t` is the only possible variable of the expression `make_periodic`, then its third argument `t` can be omitted.

- `shift(u, s, t)`
 - It returns a function of `t` that, for any given value of `t`, evaluates to the same values as `u` does when evaluated at `s` minutes before `t`.
 - `s` is the numeric value of the shift in minutes.

Note:

If `t` is the only possible variable of the expression `shift`, then its third argument `t` can be omitted.

Chapter 6: Input Commands

Command Syntax

- For position-dependent expressions:
 - The strings `x`, `y`, and `z` denote the numeric value of the `x`-, `y`-, and `z`-coordinates of a point in micrometers, respectively.
 - The strings `x<unit>`, `y<unit>`, and `z<unit>` denote the numeric value of the `x`-, `y`-, and `z`-coordinates of a point in the specified unit (possible values for `<unit>` are `m`, `um`, and `nm`), respectively.
 - `make_periodic(u, p, position)`
 - `position` can be `x` or `y` or `z`.
 - It returns a periodic function of `position` with period `p` micrometers. The returned periodic function evaluates to the same values as `u` does for $0 \leq \text{position} < p$.
 - `p` is the numeric value of the period in micrometers. It must be a nonnegative value.
 - `shift(u, s, position)`
 - `position` can be `x` or `y` or `z`.
 - It returns a function of `position` that, for any given value of `position`, evaluates to the same values as `u` does when evaluated at `position - s` micrometers.
 - `s` is the numeric value of the shift in micrometers.
- For angle-dependent expressions, the string `theta` denotes the angle in radians between the normal to the surface at the collision point and the direction of the incoming particle.
- For energy-dependent expressions, the string `E` denotes the energy in electron volts of the incoming particle.

The arguments `duty_cycle`, `period`, `v_off`, `v_on`, `u`, `v`, and `w` of these functions are themselves expressions.

A condition is an expression that can also contain relational operators:

`<`, `<=`, `>`, `>=`, `==`, `!=`

Chapter 6: Input Commands

Command Syntax

Summary of Available Commands

Table 8 *Summary of Sentaurus Topography 3D commands*

Command	Function
add_bulk_reaction	Adds a new plasma bulk reaction to a specified plasma model.
add_event	Adds an event to the list of events specified in the surface transport model.
add_float_parameter	Adds a new user-defined parameter for floating-point values to the specified rate formula module (RFM) model.
add_flux_properties	Specifies the values of the parameters for a flux associated with an RFM model.
add_formula	Defines a formula for calculating the deposition or etching rate for an RFM model.
add_int_parameter	Adds a new user-defined parameter for integer values to the specified RFM model.
add_interface_layer	Adds a layer across the interface between two materials, where a material-dependent parameter can take position-dependent values, and specifies the spatially dependent values of that parameter in that layer.
add_ion_flux	Adds a new ion flux to the specified RFM model.
add_litho_command	Adds a Sentaurus Lithography Tcl command.
add_material	Specifies the values of the parameters of an etch machine for a particular material.
add_neutral_flux	Adds a new neutral flux to the specified RFM model.
add_reaction	Adds a reaction to a reaction model.
add_reaction_properties	Specifies the values of the parameters for a reaction.
add_source_species	Adds a species to the source of a reaction model.
add_species	Adds a new plasma species to a specified plasma model.
add_volumetric_source_species	Adds a species to the volumetric source of a reaction model.

Chapter 6: Input Commands

Command Syntax

Table 8 Summary of Sentaurus Topography 3D commands (Continued)

Command	Function
define_boundary_conditions	Specifies the boundary conditions to be used when processing a structure.
define_bulk_solver	Defines the numeric parameters of the solver used to simulate the plasma bulk.
define_charging_model	Defines a charging model.
define_damage	Defines the parameters of the damage model for PMC simulations.
define_deposit_machine	Defines a machine for a built-in or an RFM deposition model.
define_diffuse_machine	Defines a machine for a diffusion process modeling voids.
define_electric_contact	Defines an electric contact.
define_electric_solver	Defines an electric solver.
define_etch_machine	Defines a machine for an etching model, or a simultaneous etching and deposition model, or a deposition reaction model.
define_extraction	Defines extractions that can be used during a deposition step or an etching step.
define_iad	Defines an ion angular distribution (IAD).
define_layout	Reads a GDSII, an OASIS®, or a TCAD layout file, which can then be used to create logical masks with the define_mask command.
define_litho_machine	Defines a machine for a lithographic process.
define_mask	Defines a mask to be used in an etch step or a patterning step.
define_material_replacement	Defines a material replacement map.
define_model	Starts the definition of a new RFM model or a new reaction model.
define_nad	Defines a neutral angular distribution (NAD).

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Command Syntax

Table 8 Summary of Sentaurus Topography 3D commands (Continued)

Command	Function
define_pattern_density	Defines a new pattern density object or extends the definition of an existing pattern density object.
define_pattern_density_model	Defines a defines a new pattern density model.
define_plasma_model	Defines a new plasma model.
define_probability	Defines an energy- and angle-dependent probability that can be used in a reaction model.
define_reactor	Defines the reactor parameters for a plasma model.
define_reflection	Defines the properties of a new reflection function.
define_shape	Defines a new shape for a geometric etch or deposit step.
define_sheath_solver	Defines the numeric parameters of the solver used to simulate the plasma sheath.
define_species_distribution	Defines the angular distribution of a source species of a reaction model.
define_species_properties	Defines the properties of a species used in a reaction model.
define_structure	Defines the initial 2D or 3D boundary structure.
define_surface_transport_model	Defines a surface transport model.
define_volumetric_species_distribution	Defines the spatial distribution of a volumetric source species of a reaction model.
define_yield	Defines the properties of a new yield function.
deposit	Performs a deposition process step on a structure.
diffuse	Performs a diffusion process step on a structure.
etch	Performs an etching process step or a simultaneous etching and deposition process step on a structure, or performs a deposition step based on a reaction model.
extend_structure	Extends a structure by mirroring it, or by copying and shifting it.

Chapter 6: Input Commands

Command Syntax

Table 8 *Summary of Sentaurus Topography 3D commands (Continued)*

Command	Function
extract	Extracts properties from a structure.
fill	Fills the structure with one or more materials.
filter_structure	Executes Boolean operations, or converts a boundary structure to a PMC structure, or converts a PMC structure to a boundary structure, or creates a copy of an existing structure, or decimates the number of surface elements, or merges several regions into one region, or creates a structure with a different surface discretization, or removes parts that are disconnected or that fit user-specified criteria, or removes a region from a structure, or renames a region of a structure, or replaces the material of the regions of a structure, or smooths a structure.
finalize_model	Indicates that the definition of a model is completed.
layout	Queries the properties of a layout that has been created with the <code>define_layout</code> command.
let	Defines global settings for Sentaurus Topography 3D.
litho	Performs a lithography simulation and adds a resist region.
pattern	Performs a patterning step on a structure.
remove_material	Removes a specified material from a structure.
save	Saves a structure, or an ion angular distribution (IAD), or a probability function, or a reflection function, or a neutral angular distribution (NAD), or pattern density-related functions, or a yield function to a TDR file, or saves a species distribution to a TDR file or to a text file, or saves a PMC structure to a PMC file, or saves a grid containing the volume fractions of the species in a PMC structure to a TDR file.
set_field	Sets the values of a field.
set_material_properties	Sets or changes the properties of materials.
set_orientation	Sets or changes the crystal orientation of a region.

Chapter 6: Input Commands

Command Syntax

Table 8 Summary of Sentaurus Topography 3D commands (Continued)

Command	Function
solve_reactor	Executes the plasma model solvers.
transform_structure	Performs an axis-mapping transformation.
truncate	Truncates a structure.

Chapter 6: Input Commands

add_bulk_reaction

add_bulk_reaction

This command adds a new plasma bulk reaction to a specified plasma model.

Note:

If you specify an `add_bulk_reaction` command with the name of a plasma bulk reaction that already exists, then this command is ignored.

Syntax

```
add_bulk_reaction a=<n> b=<n> c=<n> [d=<n> e=<n> f=<n> g=<n>] \
    energy_transfer=<n> expression=<c> name=<c> \
    plasma_model=<c> rate_coefficient_type=<c> [T_ref=<n>]
```

Table 9 Parameters of `add_bulk_reaction` command

Parameter	Description
a	<p>Sets an Arrhenius law coefficient. The unit is as follows:</p> <ul style="list-style-type: none">• none: For reactions of <code>rate_coefficient_type=general_arrhenius</code>• 1/s: For one-body reactions of <code>rate_coefficient_type=arrhenius</code>• m³/s: For two-body reactions of <code>rate_coefficient_type=arrhenius</code> <p>Type: Number Default: none Range: [0, +∞[Unit: none, or 1/s, or m³/s</p>
b	<p>Sets an Arrhenius law coefficient for any value of the <code>rate_coefficient_type</code> parameter.</p> <p>Type: Number Default: none Range:]-∞, +∞[</p>
c	<p>Sets an Arrhenius law coefficient:</p> <ul style="list-style-type: none">• For <code>rate_coefficient_type=arrhenius</code>, the unit is eV.• For <code>rate_coefficient_type=general_arrhenius</code>, no unit is specified for the coefficient. <p>Type: Number Default: none Range:]-∞, +∞[Unit: none or eV</p>

Chapter 6: Input Commands

add_bulk_reaction

Table 9 Parameters of add_bulk_reaction command (Continued)

Parameter	Description
d	Sets an Arrhenius law coefficient for <code>rate_coefficient_type=general_arrhenius</code> . Type: Number Default: 0 Range: $]-\infty, +\infty[$
e	Sets an Arrhenius law coefficient for <code>rate_coefficient_type=general_arrhenius</code> . Type: 0 Default: none Range: $]-\infty, +\infty[$
f	Sets an Arrhenius law coefficient for <code>rate_coefficient_type=general_arrhenius</code> . Type: Number Default: 0 Range: $]-\infty, +\infty[$
g	Sets an Arrhenius law coefficient for <code>rate_coefficient_type=general_arrhenius</code> . Type: Number Default: 0 Range: $]-\infty, +\infty[$
energy_transfer	Sets the energy transferred during the reaction. The following sign conventions apply: <ul style="list-style-type: none"> • Positive for endothermal reactions • Negative for exothermal reactions Type: Number Default: none Range: $]-\infty, +\infty[$ Unit: eV
expression	Sets the expression of the reaction added to the plasma model. Type: Character Default: none
name	Sets the name of the reaction. The name is used as a unique label for this reaction. Type: Character Default: none

Chapter 6: Input Commands

add_bulk_reaction

Table 9 Parameters of add_bulk_reaction command (Continued)

Parameter	Description
plasma_model	Sets the name of the plasma model to which the reaction is added. It must be already defined by define_plasma_model on page 298 . Type: Character Default: none
rate_coefficient_type	Sets the mathematical form of the rate coefficient. Options are: <ul style="list-style-type: none">• arrhenius: $a\left(\frac{T_e}{T_{ref}}\right)^b \exp\left(-\frac{c}{T_e}\right)$• general_arrhenius: $\exp\left(a + b \ln T_e + \frac{c}{T_e} + \frac{d}{T_e^2} + \frac{e}{T_e^3} + f \cdot T_e + g \cdot T_e^2\right)$ where T_e is the electron temperature in eV Type: Character Default: none
T_ref	Sets an Arrhenius law coefficient for rate_coefficient_type=arrhenius. Type: Number Default: 1 Range: [0, +∞[Unit: eV

Plasma Bulk Reactions

A plasma bulk reaction specifies a rule to transform a set of reactants into a set of products. A reaction expression must be given in the following format:

<R1> = n1<P1> + n2<P2> + ...

or:

<R1> + <R2> = n1<P1> + n2<P2> + ...

where:

- <R1> and <R2> are the species names of the reactants (that is, the state before the reaction). The number of reactants must be one or two.
- <P1>, <P2>, ... are the species names of the reaction products (that is, the state after the reaction). The number of products is arbitrary.

Chapter 6: Input Commands

add_bulk_reaction

- n1, n2, ... are the stoichiometric coefficients of the reaction products and must be positive integers. If you do not specify the stoichiometric coefficient, the default value of 1 is assumed.
- Each species name used in a reaction expression must have been previously defined within the specified model by the `add_species` command.
- The left-hand side (reactants) and the right-hand side (products) of the reaction expression are separated by an equal sign (=) with space on either side of the equal sign, and the different species on either side of the expression are separated by a plus sign (+) with space on either side of the plus sign.
- The species name `e-` is reserved for electrons, which are implicitly defined in the plasma model and, therefore, do not have to be defined explicitly by the `add_species` command.

Note:

Rate coefficients must be given in the form of an Arrhenius law:

$$r = a \text{ <m}^3/\text{s>} \cdot \left(\frac{T_e}{1 \text{ <eV>}} \right)^b \exp\left(-\frac{c \text{ <eV>}}{T_e}\right)$$

where the parameters a , b , and c are given for the electron temperature T_e in eV, and $T_{\text{ref}} = 1 \text{ eV}$. If, instead, you want to specify the parameters a , b , and c for the electron temperature T_e in K, then you must set $T_{\text{ref}} = 1 \text{ K}$:

$$r = a \text{ <m}^3/\text{s>} \cdot \left(\frac{T_e}{1 \text{ <K>}} \right)^b \exp\left(-\frac{c \text{ <K>}}{T_e}\right)$$

If you want to plot the rate coefficients, then you can use the `save` command to write the rate coefficient curve as a function of the electron temperature to a TDR file.

Examples

If the reaction coefficients are given for T_e in units of eV:

```
add_bulk_reaction plasma_model=M name=r1 \
    expression="Ar + e- = Ar+ + 2e-" \
    rate_coefficient_type=arrhenius energy_transfer=16<eV> \
    a=2e-14<m^3/s> b=0.6 c=16<eV> T_ref=1<eV>
```

If data is given for T_e in kelvin instead of eV:

```
add_bulk_reaction plasma_model=M name=r1 \
    expression="Ar + e- = Ar+ + 2e-" \
    rate_coefficient_type=arrhenius energy_transfer=16<eV> \
    a=6e-17<m^3/s> b=0.6 c=186400<K> T_ref=1<K>
```

Chapter 6: Input Commands

add_event

add_event

This command adds an event to the list of events specified in the surface transport model (see [Surface Transport Model on page 92](#)).

Syntax

Define an adsorption event:

```
add_event type=adsorption model=<c> r=<n> \
           [material=<c>] [product=<c>] [species=<c>]
```

Define a desorption event:

```
add_event type=desorption model=<c> r=<n> tracked=<b> \
           [material=<c>] [product=<c>] [species=<c>]
```

Define a deposition event:

```
add_event type=deposition model=<c> r=<n> \
           [diamond_r_<hkl>] [material=<c>] \
           [max_product_coverage=<n>] [product=<c>] [species=<c>]
```

Define a diffusion event:

```
add_event type=diffusion model=<c> \
           (diffusivity=<n> | (hopping_distance=<n> r=<n>)) \
           [material=<c>] [species=<c>]
```

Define a nucleation event:

```
add_event type=nucleation model=<c> crystal_type=<c> r=<n> \
           [material=<c>] [product=<c>] [species=<c>]
```

Define an attachment to a grain event:

```
add_event type=attachment model=<c> grain=<c> r=<n> \
           [diamond_r_<hkl>] [material=<c>] [species=<c>]
```

Chapter 6: Input Commands

add_event

Table 10 Parameters of add_event command

Parameter	Description
crystal_type	Sets the crystal type of the deposited nucleus. Type: Character Default: diamond
diamond_r_<hkl>	Sets the rate to be used for a deposition or an attachment event when the surface has a diamond crystal structure and its exposed surface is parallel to an $(h k l)$ crystal plane, where $<hkl>$ is 100 or 110 or 111. Type: Character Default: none Range: [0, ∞[Unit: s^{-1}
diffusivity	Sets the diffusivity of the adatom. This parameter is available only for type=diffusion for which either diffusivity or r can be specified. Type: Number Default: none Range: [0, ∞[Unit: cm^2/s
grain	Sets the name of the species to which the existing grain attaches. Type: Character Default: none
hopping_distance	Sets the distance between the lattice sites between which the adatom hops during the diffusion process. This parameter is available only for type=diffusion and if a rate is given. Type: Number Default: none Unit: μm
material	Specifies the surface material on which the event is defined. If this parameter is not set, then the event applies to all materials for which no material-specific events are defined. Type: Character Default: none
max_product_coverage	Sets the maximum coverage that can be reached with this event. This parameter is available only for type=deposition. Type: Number Default: 1 Range: [0, 1]

Chapter 6: Input Commands

add_event

Table 10 Parameters of add_event command (Continued)

Parameter	Description
model	Specifies the unique name of a surface transport model, defined by the define_surface_transport_model command (see define_surface_transport_model on page 365). Type: Character Default: none
product	Sets the product species of an event. This parameter is available for the following event types: <ul style="list-style-type: none">• adsorption• deposition• desorption• nucleation Type: Character Default: none
r	Sets the rate of the specified event. For type=diffusion, you can specify the diffusivity instead. Type: Number Default: none Range: [0, ∞[Unit: s ⁻¹
species	Sets the species name of the adatom for which this event should apply. If this parameter is not set, then the event applies to all surface transport species for which no specific events are defined. Type: Character Default: none
tracked	Specifies whether to track the desorbed gaseous product. This parameter is available for type=desorption. Type: Boolean Default: false

Chapter 6: Input Commands

add_event

Table 10 Parameters of add_event command (Continued)

Parameter	Description
type	Sets the type of the event. Possible types are: <ul style="list-style-type: none">• adsorption• attachment• deposition• desorption• diffusion• nucleation Type: Character Default: none

Description

When using the `add_event` command:

- For each adatom species, an event must be defined that stops surface transport. This can be any event except diffusion; otherwise, the adatom will continue to diffuse forever.
- For each event, a rate (or for `type=diffusion`, a diffusivity) must be specified, as the surface transport model randomly chooses an event according to the rates of the events.
- Every event can be specified for a specific adatom species and for a specific surface material: `add_event species=<c> material=<c> ...`

You also can define generic events that apply to all adatom species or to all surface materials for which no events are explicitly specified (fallback events). You can define generic events in different ways:

- You can define events for a specific adatom species to be applied to all materials: `add_event species=<c> ...`
- You can define events for a specific surface material to be applied to all adatom species: `add_event material=<c> ...`
- In addition, you can define a fallback event to be applied to all materials and to all adatoms for which no events are defined: `add_event ...`

Fallback events are considered only if there are no other events defined explicitly for that adatom species and for that surface material. Therefore, for clarity, it is recommended to always specify explicitly the surface material and adatom species for which an event should be applied.

Chapter 6: Input Commands

add_event

- When an adatom species A diffuses along the surface material S, the events to be executed are handled in the following order of priority:
 1. If events are defined for both the specific surface material S and the specific adatom species A, then only these events are considered, that is, they take first precedence.
 2. If events are defined for the specific adatom species A but not for a specific surface material, then only these events are considered, that is, they take second precedence.
 3. If events are defined for the specific surface material S but not for a specific adatom species, then only these events are considered, that is, they take third precedence.
 4. If events are defined without either a specific surface material or a specific adatom species, then only these events are considered, that is, they take fourth precedence.

Examples

See [Surface Transport Model on page 92](#).

Chapter 6: Input Commands

add_float_parameter

add_float_parameter

This command adds a new user-defined parameter for floating-point values to the specified RFM model.

For parameters defined as globally valid:

- You must specify the parameter `default` when `optional=true`.
The value specified with `default` is used when `optional=true` and the parameter has not been set explicitly with the `define_deposit_machine` or `define_etch_machine` command (see [define_deposit_machine on page 220](#) and [define_etch_machine on page 242](#)).
- You must not specified the parameter `default` when `optional=false`.

For material-dependent parameters, you must set the parameter `default` independently of the value of the `optional` parameter. The value specified with `default` is used for materials for which parameters have not been specified with the `add_material` command. The value is also used if `optional=true` and the parameter has not been set explicitly with the `add_material` command (see [add_material on page 177](#)).

Syntax

For deposition:

```
add_float_parameter default=<n> model=<c> name=<n> quantity=<c> \
[description=<c>] [max=<n>] [min=<n>] [optional=<c>]
```

For etching and simultaneous etching and deposition:

```
add_float_parameter default=<n> model=<c> name=<n> quantity=<c> \
scope=<c> [description=<c>] [max=<n>] [min=<n>] [optional=<c>]
```

Table 11 Parameters of add_float_parameter command

Parameter	Description
default	Sets the default value to assign to the new parameter for unknown materials and also if the new parameter is optional. Type: Number Default: none Unit: Default unit of quantity set by <code>quantity</code> parameter
description	Describes the new parameter. Type: Character Default: empty string

Chapter 6: Input Commands

add_float_parameter

Table 11 Parameters of add_float_parameter command (Continued)

Parameter	Description
max	Sets the maximum value of the new parameter. Use the <code>max</code> and <code>min</code> parameters to limit the valid range of the new parameter. Type: Number Default: ∞ Unit: Default unit of quantity set by <code>quantity</code> parameter
min	Sets the minimum value of the new parameter. Use the <code>max</code> and <code>min</code> parameters to limit the valid range of the new parameter. Type: Number Default: $-\infty$ Unit: Default unit of quantity set by <code>quantity</code> parameter
model	Sets the RFM model to which the new parameter is added. Note: The <code>model</code> parameter must specify an RFM model, that is, the <code>type</code> parameter must have been set in the <code>define_model</code> command for that model (see define_model on page 289). Type: Character Default: none
name	Sets the name of the new parameter. When <code>scope=global</code> , these values cannot be used: <code>applied_pressure</code> , <code>deposit_material</code> , <code>iad</code> , <code>material</code> , <code>maximum_error</code> , <code>model</code> , <code>name</code> , <code>pad_poisson_ratio</code> , <code>pad_roughness</code> , <code>pad_yang_modulus</code> , <code>reflection</code> , <code>rotation</code> , <code>tilt</code> , <code>yield</code> When <code>scope=material_dependent</code> , the value <code>material</code> cannot be used. Type: Character Default: none
optional	Specifies whether the new parameter is optional when the model is used. Note: In general, do not make a parameter optional. Instead, simplify a model to such a degree that all user-defined parameters are required. Type: Boolean Default: false

Chapter 6: Input Commands

add_float_parameter

Table 11 Parameters of add_float_parameter command (Continued)

Parameter	Description
quantity	<p>Sets the physical quantity of the new parameter value. The expression for the rate defined with the <code>add_formula</code> command must have the dimension of a velocity (see add_formula on page 164). Options are:</p> <ul style="list-style-type: none">• angle (default unit: degree)• dimensionless (default unit: 1)• energy (default unit: eV)• length (default unit: μm)• time (default unit: minute)• velocity (default unit: μm/minute) <p>Type: Character Default: none</p>
scope	<p>Sets how the new parameter is defined. Options are:</p> <ul style="list-style-type: none">• global: New parameter is valid globally.• material_dependent: New parameter is material dependent. <p>This parameter applies only to etching and simultaneous etching and deposition. Type: Character Default: none</p>

Examples

Add a parameter for a deposition model:

```
define_model description="Advanced CVD model" name=depo_CVD \
    type=deposit

    add_float_parameter default=12 model=depo_CVD name=tilt \
        quantity=angle description="Irrational tilt angle" min=5 max=45
```

The `model` parameter is dependent on specifying the `type` parameter in the `define_model` command beforehand. In this example, since `quantity=angle`, the default unit for the `default`, `max`, and `min` parameters is degree.

Add a parameter for an etching model:

```
define_model description="Modified RIE model" name=etch_rie \
    type=etch

    add_float_parameter default=2 model=etch_rie name=sim_time \
        quantity=time scope=global
```

The `model` parameter is dependent on specifying the `type` parameter in the `define_model` command beforehand. In this example, since the new parameter is for an etching model, the `scope` parameter is required.

Chapter 6: Input Commands

add_flux_properties

add_flux_properties

This command specifies the parameters of a flux associated with an RFM model. There are different forms of the command for neutral and ion fluxes.

Syntax

For neutral fluxes, you must specify the value of the sticking coefficient. For deposition models, the sticking coefficient is material independent (otherwise, it is material dependent):

```
add_flux_properties flux=<c> sticking=<n> [machine=<c>]  
add_flux_properties flux=<c> material=<c> sticking=<n> [machine=<c>]
```

If `sputter_deposition` has been activated for an ion flux during the model definition (see [add_ion_flux on page 174](#)), then the values for the parameters `sputter_exponent` (exponent of the angular distribution of the emission of the sputtered material), `sputter_type` (the type of emission of the sputtered material), and `sticking` (the sticking coefficient of the reemitted material) must be specified. Otherwise, these parameters must not be specified.

For ion fluxes, in deposition models, the flux parameters are material independent; whereas, for etching and simultaneous etching and deposition, they are material dependent:

```
add_flux_properties flux=<c> [machine=<c>] [sputter_exponent=<n>] \  
[sputter_type=<c>] [sticking=<n>]  
  
add_flux_properties flux=<c> material=<c> [machine=<c>] \  
[sputter_exponent=<n>] [sputter_type=<c>] [sticking=<n>]
```

The `flux` parameter takes the name that was given to a flux in the model definition with the `add_neutral_flux` or `add_ion_flux` command.

Note:

If `sputter_exponent`, `sputter_type`, or `sticking` has been fixed in the model definition (given a constant value), then you cannot specify the parameter again with the `add_flux_properties` command.

Table 12 Parameters of `add_flux_properties` command

Parameter	Description
flux	Sets the name of the flux to configure. Type: Character Default: none

Chapter 6: Input Commands

add_flux_properties

Table 12 Parameters of add_flux_properties command (Continued)

Parameter	Description
machine	<p>Sets the name of the machine for which the flux is configured.</p> <p>Note: The <code>machine</code> parameter must specify a machine using an RFM model, that is, the <code>type</code> parameter must have been set in the <code>define_model</code> command for that model (see define_model on page 289).</p> <p>Type: Character Default: <code>default_machine</code></p>
material	<p>Sets the material for which the properties are specified.</p> <p>Type: Character Default: none</p>
sputter_exponent	<p>Sets the exponent used to characterize the angular distribution $\cos^m\theta$ of the sputtered material. The value must be an integer.</p> <p>Type: Number Default: none Range: $[1, \infty[$</p>
sputter_type	<p>Sets the sputter reemission type of the model (see add_ion_flux on page 174). Options are:</p> <ul style="list-style-type: none"> • diffuse • reflective <p>Type: Character Default: none</p>
sticking	<p>Sets the sticking coefficient.</p> <p>Type: Number Default: none Range: $[0, 1]$</p>

Examples

```
# Define a model with sputter deposition activated that fixes
# the sputter exponent and type, but not the sticking.
define_model name=m type=deposit description=""

add_ion_flux model=m name=i energy=independent reflection=false \
    sputtering=true sputter_deposition=true sputter_exponent=1 \
    sputter_type=diffuse

add_formula model=m expression="sputter_depo_flux(i)-direct_flux(i)"
```

Chapter 6: Input Commands

add_flux_properties

```
finalize_model model=m

# ...
# When model is used:
define_deposit_machine model=m material=Oxide ...

# OK: Parameter sticking is required because sputter deposition is
# switched on in the model definition.
add_flux_properties model=m flux=i sticking=0.9

# Error: sputter_exponent has a constant value of 1 and cannot be
# specified again here when model is used.
add_flux_properties model=m flux=i sputter_exponent=100 sticking=0.9
```

Chapter 6: Input Commands

add_formula

add_formula

This command defines the formula for calculating the deposition or etching rate. To make it easier to develop and maintain an RFM model, you can define subexpressions and use them in the definition of subsequent subexpressions and the main expression for the rate.

For etching and simultaneous etching and deposition, there is a material independent form and material dependent form of the `add_formula` command:

- The material-independent form defines a default rate formula. The default rate formula is used for all materials for which no specific rate formula has been defined.
- The material-dependent form defines a rate formula for a specific material.

[Rate Calculation on page 572](#) describes the data and functions available for defining the formula for the rate. In addition, previously defined subexpressions can be used as part of the new rate formula.

Syntax

For deposition and for default rate formulas (material-independent form):

```
add_formula model=<c> name=<c> subexpression=<c> [unit=<c>]
```

```
add_formula expression=<c> model=<c> [unit=<c>]
```

For material-dependent rate formulas:

```
add_formula material=<c> model=<c> name=<c> subexpression=<c> [unit=<c>]
```

```
add_formula expression=<c> material=<c> model=<c> [unit=<c>]
```

Table 13 Parameters of `add_formula` command

Parameter	Description
expression	Sets the formula used to calculate the rate. Type: Character Default: none
material	Sets the material for which the formula is used. Type: Character Default: none

Chapter 6: Input Commands

add_formula

Table 13 Parameters of *add_formula* command (Continued)

Parameter	Description
model	Sets the RFM model to which the formula is added. Note: The <code>model</code> parameter must specify an RFM model, that is, the <code>type</code> parameter must have been set in the <code>define_model</code> command for that model. Type: Character Default: none
name	Sets the name of the subexpression. Type: Character Default: none
subexpression	Sets the formula used to calculate the subexpression. Type: Character Default: none
unit	Sets the unit of the expression or subexpression. Options are: <ul style="list-style-type: none">• nm min⁻¹• nm s⁻¹• um min⁻¹• um s⁻¹ Type: Character Default: um min ⁻¹

Chapter 6: Input Commands

add_int_parameter

add_int_parameter

This command adds a new user-defined parameter for integer values to the specified RFM model.

For parameters defined as globally valid:

- You must specify the parameter `default` when `optional=true`.
The value specified with `default` is used when `optional=true` and the parameter has not been set explicitly with the `define_deposit_machine` or `define_etch_machine` command (see [define_deposit_machine on page 220](#) and [define_etch_machine on page 242](#)).
- You must not specified the parameter `default` when `optional=false`.

For material-dependent parameters, you must set the parameter `default` independently of the value of the `optional` parameter. The value specified with `default` is used for materials for which parameters have not been specified with the `add_material` command. The value is also used if `optional=true` and the parameter has not been set explicitly with the `add_material` command (see [add_material on page 177](#)).

Syntax

For deposition:

```
add_int_parameter default=<n> model=<c> name=<c> \
[description=<c>] [max=<n>] [min=<n>] [optional=<c>]
```

For etching and simultaneous etching and deposition:

```
add_int_parameter default=<n> model=<c> name=<c> scope=<c> \
[description=<c>] [max=<n>] [min=<n>] [optional=<c>]
```

Table 14 Parameters of `add_int_parameter` command

Parameter	Description
<code>default</code>	Sets the default value to assign to the new parameter for unknown materials and also if the new parameter is optional. Type: Number Default: none
<code>description</code>	Describes the new parameter. Type: Character Default: empty string

Chapter 6: Input Commands

add_int_parameter

Table 14 Parameters of add_int_parameter command (Continued)

Parameter	Description
max	<p>Sets the maximum value of the new parameter. Use the <code>max</code> and <code>min</code> parameters to limit the valid range of the new parameter.</p> <p>Type: Number Default: 2147483647 Range: [-2147483648, 2147483647]</p>
min	<p>Sets the minimum value of the new parameter. Use the <code>max</code> and <code>min</code> parameters to limit the valid range of the new parameter.</p> <p>Type: Number Default: -2147483647 Range: [-2147483648, 2147483647]</p>
model	<p>Sets the RFM model to which the integer parameter is added.</p> <p>Note: The <code>model</code> parameter must specify an RFM model, that is, the <code>type</code> parameter must have been set in the <code>define_model</code> command for that model (see define_model on page 289).</p> <p>Type: Character Default: none</p>
name	<p>Sets the name of the new parameter.</p> <p>When scope=global, these values cannot be used: applied_pressure, deposit_material, iad, material, maximum_error, model, name, pad_poisson_ratio, pad_roughness, pad_young_modulus, reflection, rotation, tilt, yield</p> <p>When scope=material_dependent, the material value cannot be used.</p> <p>Type: Character Default: none</p>
optional	<p>Specifies whether the new parameter is optional when the model is used.</p> <p>Note: In general, do not make a parameter optional. Instead, simplify a model to such a degree that all user-defined parameters are required.</p> <p>Type: Boolean Default: false</p>

Chapter 6: Input Commands

add_int_parameter

Table 14 *Parameters of add_int_parameter command (Continued)*

Parameter	Description
scope	<p>Sets how the new parameter is defined. Options are:</p> <ul style="list-style-type: none">• <code>global</code>: New parameter is valid globally.• <code>material_dependent</code>: New parameter is material dependent. <p>The <code>scope</code> parameter applies only to etching and simultaneous etching and deposition.</p> <p>Type: Character Default: none</p>

Chapter 6: Input Commands

add_interface_layer

add_interface_layer

This command adds a layer across the interface between two different materials, where a numeric material-dependent parameter can take position-dependent values, and specifies the spatially dependent values of that parameter in that layer.

Note:

The `add_interface_layer` command can be used only for machines using level set-based models. This command cannot be used for deposition machines or for machines using simultaneous etching and deposition models.

When using a built-in model, the `add_interface_layer` command is not supported for the sticking and reflection parameters.

This command uses the initial structure to determine the spatially dependent parameter values and has different versions.

Syntax

For a linear grading of the specified parameter across the interface between its bulk values, which are specified with the `add_material` command:

```
add_interface_layer material1=<c> material2=<c> parameter=<c> \
thickness1=<n> thickness2=<n> [machine=<c>]
```

For a piecewise linear grading of the specified parameter across the interface between its bulk values, which are specified with the `add_material` command:

```
add_interface_layer material1=<c> material2=<c> parameter=<c> \
table1=<v> table2=<v> \
[machine=<c>] [table1_distance_unit=<c>] [table2_distance_unit=<c>]
```

Table 15 Parameters of `add_interface_layer` command

Parameter	Description
machine	Sets the name of the machine to which an interface layer is added. Type: Character Default: default_machine
material1	Sets the name of the first material of the interface. It must be a material different from the material specified with <code>material2</code> . Type: Character Default: none

Chapter 6: Input Commands

add_interface_layer

Table 15 Parameters of add_interface_layer command (Continued)

Parameter	Description
material2	Sets the name of the second material of the interface. It must be a material different from the material specified with material1. Type: Character Default: none
parameter	Sets the name of the material-dependent parameter for which an interface layer is specified. The name must be one of the material-dependent parameter names of the machine specified by machine. For RFM models, it must be one of the parameters defined using the add_float_parameter command. Type: Character Default: none
table1	Sets the tabular format of the piecewise linear scaling of the parameter value in the region of space occupied by the material specified by material1 (see Tabular Format on page 171). Type: Vector Default: none
table1_distance_unit	Sets the unit of distances listed in table1. Options are: <ul style="list-style-type: none">• nm• m• um Type: Character Default: um
table2	Sets the tabular format of the piecewise linear scaling of the parameter value in the region of space occupied by the material specified by material2 (see Tabular Format on page 171). Type: Vector Default: none
table2_distance_unit	Sets the unit of distances listed in table2. Options are: <ul style="list-style-type: none">• nm• m• um Type: Character Default: um

Chapter 6: Input Commands

add_interface_layer

Table 15 Parameters of add_interface_layer command (Continued)

Parameter	Description
thickness1	Sets the thickness of the interface layer in the region of space occupied by the material specified by material1. Type: Number Default: none Range: [0, ∞[Unit: μm
thickness2	Sets the thickness of the interface layer in the region of space occupied by the material specified by material2. Type: Number Default: none Range: [0, ∞[Unit: μm

Tabular Format

The parameters table1 and table2 require a vector of numbers that fulfill the following conditions (the convention that the first vector element has index 0 is understood):

- The number of elements of the vector must be even and not less than 4.
- Vector elements with an even index represent a distance from the interface and must be nonnegative, unique, and sorted in ascending order.
- Vector elements with an odd index represent a scaling factor for the corresponding bulk value of the parameter specified with the add_material command and must be nonnegative.
- The first vector element (that is, the first distance) must be 0.
- The last vector element (that is, the last scaling factor) must be 1.

Examples

The following commands define an etch machine using the simple model, where the rate parameter values vary linearly across the interfaces between silicon and oxide:

```
define_etch_machine model=simple
add_material material=Silicon rate=1. anisotropy=0.5 curvature=0.
add_material material=Oxide rate=0.1 anisotropy=0.5 curvature=0.
add_material material=Nitride rate=0.5 anisotropy=0.5 curvature=0.
add_interface_layer material1=Silicon material2=Oxide parameter=rate \
    thickness1=0.1 thickness2=0.2
```

Chapter 6: Input Commands

add_interface_layer

In particular:

- The value of the `rate` parameter is 1 $\mu\text{m}/\text{minute}$ for points that are located in a region occupied by material `Silicon` and with a distance from a silicon–oxide interface greater than 0.1 μm .
- The value of the `rate` parameter is 0.1 $\mu\text{m}/\text{minute}$ for points that are located in a region occupied by material `Oxide` and with a distance from a silicon–oxide interface greater than 0.2 μm .
- The value of the `rate` parameter decreases linearly from 1 $\mu\text{m}/\text{minute}$ to 0.1 $\mu\text{m}/\text{minute}$ as you move along a segment that crosses the silicon–oxide interface orthogonally, starting from a point located in the silicon region at 0.1 μm from that interface and up to a point located in the oxide region at 0.2 μm from that interface.
- The value of the `rate` parameter is 0.5 $\mu\text{m}/\text{minute}$ for points located in a region occupied by material `Nitride`.

The following commands define an etch machine using an RFM model, where the `R` parameter values vary linearly across the interfaces between silicon and oxide:

```
define_model name=m type=etch description="isotropic RFM etch model"
add_float_parameter name=R model=m quantity=velocity \
    scope=material_dependent default=0
add_formula model=m expression="-R()"
finalize_model model=m

define_etch_machine model=m
add_material material=Silicon R=1
add_material material=Oxide R=2
add_interface_layer parameter=R material1=Silicon material2=Oxide \
    table1={0 0.1 1 0.5 2 1} table1_distance_unit=nm \
    table2={0 0.1 1 0.2 1.5 1} table2_distance_unit=nm
```

In particular:

- The value of the `R` parameter is 1 $\mu\text{m}/\text{minute}$ for points that are located in a region occupied by material `Silicon` and with a distance from a silicon–oxide interface greater than 2 nm.
- The value of the `R` parameter is 2 $\mu\text{m}/\text{minute}$ for points that are located in a region occupied by material `Oxide` and with a distance from a silicon–oxide interface greater than 1.5 nm.
- The value of the `R` parameter changes in a piecewise linear way from 1 $\mu\text{m}/\text{minute}$ to 2 $\mu\text{m}/\text{minute}$ as you move along a segment that crosses the silicon–oxide interface orthogonally, starting from a point located in the silicon region at 2 nm from that interface and up to a point located in the oxide region at 1.5 nm from that interface.

Chapter 6: Input Commands

add_interface_layer

- The values of the R parameter on the silicon side of the interface layer are determined by multiplying the bulk value of the R parameter (that is, 1 $\mu\text{m}/\text{minute}$) by the piecewise linear scaling factor specified by the parameter `table1`.
- The values of the R parameter on the oxide side of the interface layer are determined by multiplying the bulk value of the R parameter (that is, 2 $\mu\text{m}/\text{minute}$) by the piecewise linear scaling factor specified by the parameter `table2`.

Note:

When using the `etch` command with a machine having interface layers defined, it is recommended to set the `spacing` parameter such that the spatial changes of the parameter values can be properly resolved.

Chapter 6: Input Commands

add_ion_flux

add_ion_flux

This command adds a new ion flux to the specified RFM model.

If you activate redeposition of the sputtered material, you can use the optional parameters `sputter_exponent`, `sputter_type`, and `sticking` to define constant values for the exponent of the angular distribution of the emission of the sputtered material, the type of emission of the sputtered material, and the sticking coefficient of the reemitted material, respectively. If any of these parameters is defined with the `add_ion_flux` command, its value cannot be changed with a subsequent `add_flux_properties` command.

Syntax

```
add_ion_flux energy=<c> model=<c> name=<c> reflection=<b> \
    sputter_deposition=<b> sputtering=<b> \
    [sputter_exponent=<n>] [sputter_type=<c>] [sticking=<n>]
```

Table 16 Parameters of `add_ion_flux` command

Parameter	Description
energy	Selects whether the reflection and sputtering are energy dependent when performing flux integration, depending on the kinetic energy of the ion species. Options are: <ul style="list-style-type: none">• dependent• independent Type: Character Default: independent
model	Sets the RFM model to which the ion flux is added. Note: The <code>model</code> parameter must specify an RFM model, that is, the <code>type</code> parameter must have been set in the <code>define_model</code> command for that model. Type: Character Default: none
name	Sets the name to be given to the ion flux. This name is used to reference the ion flux when configuring the flux properties using the <code>add_flux_properties</code> command and when accessing the flux values in the formula for calculating the etching and deposition rates. Type: Character Default: none

Chapter 6: Input Commands

add_ion_flux

Table 16 Parameters of add_ion_flux command (Continued)

Parameter	Description
reflection	Specifies whether ion reflection is taken into account. Type: Boolean Default: false
sputter_deposition	Specifies whether to calculate the redeposition of sputtered material. Note: This parameter must be specified if sputtering=true. Otherwise, it must not be specified. Type: Boolean Default: none
sputter_exponent	Sets the distribution exponent of the sputtered material. Type: Number Default: none Range: [1, ∞[
sputter_type	Sets the sputter reemission type of the model. Options are: <ul style="list-style-type: none">• diffuse• reflective Type: Character Default: none
sputtering	Specifies whether to take sputtering into account. Type: Boolean Default: false
sticking	Sets the sticking coefficient. Type: Number Default: none Range: [0, 1]

Chapter 6: Input Commands

add_litho_command

add_litho_command

This command adds a Sentaurus Lithography Tcl command to a lithography machine identified by its name. A lithography machine must be created with the `define_litho_machine` command before using the `add_litho_command` command. The `machine` parameter specifies the name of the machine to which the Tcl command is added.

Note:

The `add_litho_command` command cannot be used when you start Sentaurus Topography 3D with a value greater than 1 for the command-line option `--processes` (see [From the Command Line on page 17](#)).

Users are responsible for specifying the correct parameters depending on the specified Sentaurus Lithography Tcl command.

In general, material and simulation parameters should be specified in the SLO file or the Sentaurus Lithography material database. The `add_litho_command` command should be used mainly for varying a limited number of parameters, for example, in a parameterized Sentaurus Workbench project.

Syntax

```
add_litho_command machine=<c> <slitho command> <slitho arguments>
```

Table 17 Parameters of add_litho_command command

Parameter	Description
machine	Sets the name of the lithography machine. You can use this name in subsequent <code>litho</code> commands for creating a resist region by a lithography simulation. Type: Character Default: none
<slitho command>	Sets the Sentaurus Lithography Tcl command. Type: Character Default: none
<slitho arguments>	Sets the arguments to a Sentaurus Lithography Tcl command, without the Sentaurus Lithography connection handle. Type: Character Default: none

Chapter 6: Input Commands

add_material

add_material

This command defines the material-dependent properties of an etch machine (`define_etch_machine`), and it can be used several times for the same etch machine to configure the properties of different materials. A material cannot be configured with the `add_material` command more than once.

The machine to be configured is referenced with the `machine` parameter that must match one of the names of the previously defined etch machines.

Note:

The `add_material` command is not supported by etching machines having `model=crystal` because it is not needed. The properties of the material etched by an etching machine having `model=crystal` are set using the `define_etch_machine` command. The crystallographic orientation of the regions containing the material etched by an etching machine having `model=crystal` can be set with the command `set_orientation`. See [Orientation-Dependent Models on page 56](#), [Crystallographic Orientation-Dependent Etching on page 77](#), [define_etch_machine on page 242](#), and [set_orientation on page 547](#).

The `add_material` command is not supported by etching machines using reaction models because it is not needed. In fact, reaction models use reactions to specify material-dependent behavior. The properties of reactions are set using the `add_reaction_properties` command (see [add_reaction_properties on page 188](#)).

Syntax

Simple etching:

```
add_material anisotropy=<n> curvature=<n> material=<c> rate=<n> \
[machine=<c>]
```

Dry etching:

```
add_material material=<c> rate=<n> s1=<n> s2=<n> [machine=<c>]
```

Wet etching:

```
add_material material=<c> rate=<n> [deactivation_rate=<n>] \
[density=<n>] [machine=<c>]
```

Simultaneous etching and deposition (etchdepo):

```
add_material material=<c> rate=<n> s1=<n> s2=<n> [machine=<c>] \
[sputter_type=<c>] [reflection=<n>]
```

Chapter 6: Input Commands

add_material

Simultaneous etching and deposition 2 (etchdepo2):

```
add_material anisotropy=<n> material=<c> rate=<n> s1=<n> s2=<n> \
sticking=<n> [desorption_rate=<n>] [machine=<c>] [reflection=<n>]
```

High-density plasma etching:

```
add_material anisotropy=<n> material=<c> rate=<n> s1=<n> s2=<n> \
[machine=<c>]
```

High-density plasma 2 etching:

```
add_material anisotropy=<n> material=<c> rate=<n> s1=<n> s2=<n> \
sputter_rate=<n> sticking=<n> [machine=<c>] [reflection=<n>]
```

Ion-enhanced etching:

```
add_material anisotropy=<n> material=<c> rate=<n> s1=<n> s2=<n> \
sticking=<n> [desorption_rate=<n>] [machine=<c>] [reflection=<n>]
```

Ion-milling:

```
add_material anisotropy=<n> material=<c> rate=<n> s1=<n> s2=<n> \
[machine=<c>]
```

Reactive ion etching:

```
add_material anisotropy=<n> material=<c> rate=<n> [machine=<c>]
```

Reactive ion etching 2:

```
add_material anisotropy=<n> material=<c> rate=<n> sticking=<n> \
[machine=<c>] [reflection=<n>]
```

RFM model:

```
add_material material=<c> [machine=<c>] ...
```

Table 18 Parameters of add_material command

Parameter	Description
anisotropy	Sets the anisotropy coefficient for the current material. Type: Number Default: none Range: [0, 1]
curvature	Sets the curvature coefficient for the current material. Type: Number Default: none Range: [0, 0.1] Unit: µm

Chapter 6: Input Commands

add_material

Table 18 Parameters of add_material command (Continued)

Parameter	Description
deactivation_rate	Sets the rate at which etchants are deactivated when reaching the surface. Type: Number Default: 0 Range: $[0, \infty[$ Unit: $\mu\text{m min}^{-1}$
density	Sets the volume density of the current material. Type: Number Default: 1 Range: $]0, \infty[$ Unit: mol cm^{-3}
desorption_rate	Sets the thermal desorption rate for the material. Type: Number Default: 0 Range: $[0, \infty[$ Unit: $\mu\text{m min}^{-1}$
machine	Sets the machine to which the command is applied. Type: Character Default: default_machine
material	Sets the material. Type: Character Default: none
rate	Sets the etching rate for the current material. Type: Number Default: none Range: $[0, \infty[$ Unit: $\mu\text{m min}^{-1}$
reflection	Sets the reflection parameter used to evaluate the reflection probability [1]. Type: Number Default: 0 Range: $[0, 1]$
s1	Sets the first sputter coefficient. Type: Number Default: none

Chapter 6: Input Commands

add_material

Table 18 Parameters of add_material command (Continued)

Parameter	Description
s2	Sets the second sputter coefficient. Type: Number Default: none
sputter_rate	Sets the sputter rate. Type: Number Default: none Range: [0, ∞[Unit: μm min ⁻¹
sputter_type	Sets the angular distribution type of the sputtered material. The value reflective is only supported for the radiosity method for flux integration. Options are: <ul style="list-style-type: none">• diffuse• reflective Type: Character Default: diffuse
sticking	Sets the sticking coefficient. Type: Number Default: none Range: [0, 1]

Examples

This command configures the material-dependent parameters of the previously defined machine etchmachine for the material Silicon, with rate of 0.5 μm/minute, an anisotropy coefficient of 0.3, and a curvature coefficient of 0.05 μm:

```
add_material machine=etchmachine material=Silicon anisotropy=0.3 \
curvature=0.05 rate=0.5
```

Note:

For materials that are contained in the initial TDR structure, whose properties have not been defined with the add_material command, the etch rate is zero.

Chapter 6: Input Commands

add_neutral_flux

add_neutral_flux

This command adds a new neutral flux to the specified RFM model.

Syntax

```
add_neutral_flux model=<c> name=<c> [sticking=<n>]
```

Table 19 Parameters of add_neutral_flux command

Parameter	Description
model	<p>Sets the RFM model to which the neutral flux is added.</p> <p>Note: The <code>model</code> parameter must specify an RFM model, that is, the <code>type</code> parameter must have been set in the <code>define_model</code> command for that model.</p> <p>Type: Character Default: none</p>
name	<p>Sets the name of the neutral flux.</p> <p>This name is used to reference it when configuring the flux properties using the <code>add_flux_properties</code> command and when accessing the flux values in the formula for calculating the etching and deposition rates.</p> <p>Type: Character Default: none</p>
sticking	<p>Sets the sticking coefficient.</p> <p>This parameter can define a constant for the sticking coefficient. If you set this parameter, the sticking coefficient for this flux cannot be changed with a subsequent <code>add_flux_properties</code> command.</p> <p>Type: Number Default: none Range: [0, 1]</p>

Chapter 6: Input Commands

add_reaction

add_reaction

This command defines a reaction of a reaction model.

Syntax

For binary collision approximation (BCA) reactions:

```
add_reaction type=bca incoming_species=<c> \
    target_product_map=<l> target_species=<l> \
    tracked_product_species=<l>
```

For non-BCA reactions:

```
add_reaction expression=<c> model=<c> name=<c> [type=pmc]
```

Table 20 Parameters of add_reaction command

Parameter	Description
expression	Sets the expression of the reaction added to the model. Type: Character Default: none
incoming_species	Sets the name of the gas species reactant of the reaction. Applies only to BCA reactions. Type: Character Default: none
model	Sets the name of the model to which the reaction is added. Note: The <code>model</code> parameter must specify a reaction model, that is, the <code>type</code> parameter must have been set in the <code>define_model</code> command for that model. Type: Character Default: none
name	Sets the name of the reaction. Type: Character Default: none

Chapter 6: Input Commands

add_reaction

Table 20 Parameters of add_reaction command (Continued)

Parameter	Description
target_product_map	Specifies a list of pairs for those species whose type should change from <i>target</i> to <i>product</i> . The format is {target1 product1 target2 product2}. Applies only to BCA reactions. Type: List Default: none
target_species	Specifies a list of material species that are the nongas reactants of the reaction. Applies only to BCA reactions. Type: List Default: none
tracked_product_species	Specifies a list of species tracked by the simulator, which can participate in subsequent reactions. Applies only to BCA reactions. Type: List Default: none
type	Specifies the type of reaction to create (see BCA Reactions on page 95). Options are: <ul style="list-style-type: none">• bca• pmc Type: Character Default: pmc

Description

A reaction specifies a rule to transform a set of reactants into a set of products. The transformation specified by the `add_reaction` command is irreversible.

A reaction expression consists of two reaction states:

- The first reaction state describes the state *before* the reaction (specifying the *reactants*).
- The second reaction state describes the state *after* the reaction (specifying the *products*).

Reaction states are separated by the equal sign (=).

Each reaction state consists of one or more chemical species terms, which are separated by the plus sign (+). A chemical species term consists of a chemical symbol and a species-type modifier (see [Table 21](#)).

Chapter 6: Input Commands

add_reaction

Table 21 Valid species-type modifiers

Modifier	Description
<a>	Physisorbed species forming an adatom
	Bulk species
<g>	Gaseous species
<p>	Sputtered product species that is tracked by the simulator
<q>	Sputtered product species that is not tracked by the simulator
<r>	Reflected product
<s>	Surface species
<t>	Top plane species (plasma source species)
<v>	Product that is not tracked by the simulator

Limitations

The following limitations apply:

- Each reaction must have exactly two reactants: one with the <g> species-type modifier and one with the <s> or <t> species-type modifier.
- Except for top plane reactions, each reaction is allowed to have, at most, one product that goes into the reactor and that is tracked. The species-type modifiers that denote products that go into the reactor and that are tracked are <g>, <p>, and <r>.

BCA Reactions

BCA reactions model multiple interactions for each ion–material collision, and these interactions are computed automatically.

To specify a BCA reaction, use `type=bca` and specify the incoming (ion) with the `incoming_species` parameter and a list of target species using the `target_species` parameter. These two parameters determine when the BCA model is eligible to be used to compute the ion–material interaction. Specifically, when the named incoming species hits a material cell containing at least one of the named target species, the BCA model is invoked. Any material species not in the `target_species` list is unmodified by the model. Whether or not an eligible BCA reaction is called depends on the probability assigned with the `add_reaction_properties` command.

Chapter 6: Input Commands

add_reaction

Incoming species of BCA reactions can be either atomic or molecular. To specify a molecule, use the `species` and `stoichiometry` parameters of the `add_source_species` command (see [add_source_species on page 203](#)).

BCA reactions can optionally produce product species that are tracked by the simulator and that can participate in subsequent reactions or sputter events. All target species automatically become products, but those that should be tracked are specified with the `tracked_product_species` parameter. Typically, a tracked species is the same as the target species, but there is also an option to change a target species to another type when it leaves the structure if, for example, a reaction occurs. To change the species type from target to product, use the parameter `target_product_map`. All species listed in the `tracked_product_species` parameter must be in either the `target_species` list or the `target_product_map` list.

Example of Adsorption Reaction

The following command adds a reaction named `r1` to the model `reaction_model`:

```
add_reaction model=reaction_model \
    expression="F<g> + Silicon<s> = SiF<s>" name=r1
```

According to the specified expression, when an atom of species `F` coming from the reactor reacts with an atom of `Silicon` on the surface of the processed structure, a `SiF` molecule is produced. The effect of such a reaction is that a `SiF` molecule is adsorbed.

Example of Etching Reactions

The following commands add two reactions `r2` and `r3` to the model `reaction_model`:

```
add_reaction model=reaction_model \
    expression="Ar<g> + Silicon<s> = Silicon<v>" name=r2
add_reaction model=reaction_model \
    expression="Cl<g> + Silicon<s> = SiCl<g>" name=r3
```

According to reaction `r2`, when an atom of species `Ar` coming from the reactor reacts with an atom of `Silicon` on the surface of the processed structure, that silicon atom is removed without being tracked by the simulator.

According to reaction `r3`, when an atom of species `Cl` coming from the reactor reacts with an atom of `Silicon` on the surface of the processed structure, a `SiCl` molecule is produced and it goes into the reactor and is tracked by the simulator. The net effect of this reaction is that a silicon atom is etched from the structure.

Example of Deposition Reactions

The following command adds a reaction named `r4` to the model `reaction_model`:

```
add_reaction model=reaction_model \
    expression="SiH2<g> + Silicon<s> = Silicon<s> + Silicon<b> + H2<v>" \
    name=r4
```

Chapter 6: Input Commands

add_reaction

According to the specified expression, when a molecule of species `SiH2` coming from the reactor reacts with an atom of `Silicon` on the surface of the processed structure, a `Silicon` atom goes into the bulk and a new `Silicon` atom is deposited on the surface of the structure. Moreover, a `H2` molecule is produced, but it is not tracked by the simulator.

Therefore, from the perspective of the simulation, the following command is equivalent to the previous one:

```
add_reaction model=reaction_model \
    expression="SiH2<g> + Silicon<s> = Silicon<s> + Silicon<b>" name=r4
```

However, including the chemical species term `H2<v>` makes the reaction clearer and more readable.

Example of Sputtering Reactions

The following commands add two reactions `r5` and `r6` to the model `reaction_model`:

```
add_reaction model=reaction_model \
    expression="I<g> + Silicon<s> = Silicon<p>" name=r5
add_reaction model=reaction_model \
    expression="Ar<g> + Photoresist<s> = Photoresist<q>" name=r6
```

According to reaction `r5`, when an atom of species `I` coming from the reactor reacts with an atom of `Silicon` on the surface of the processed structure, a `Silicon` atom is sputtered and tracked by the simulator. Since the sputtered atom is tracked, it can be deposited somewhere if the model contains a proper reaction for silicon deposition.

According to reaction `r6`, when an atom of species `Ar` coming from the reactor reacts with an atom of `Photoresist` on the surface of the processed structure, a `Photoresist` atom is sputtered off the structure. However, the removed atom is not tracked by the simulator. As a consequence, this reaction models the sputtering of `Photoresist` by `Ar`, but it cannot be used if the deposition of the sputtered `Photoresist` must be modeled.

Example of Reflection Reaction

The following command adds a reaction named `r7` to the model `reaction_model`:

```
add_reaction model=reaction_model \
    expression="I<g> + Nitride<s> = I<r> + Nitride<s>" name=r7
```

According to reaction `r7`, when an atom of species `I` coming from the reactor reacts with an atom of `Nitride` on the surface of the processed structure, the `Nitride` atom is left untouched; whereas, the `I` atom is reflected.

Chapter 6: Input Commands

add_reaction

Example of Top Plane Reactions

The following command adds a plasma depletion reaction between gaseous surface reaction byproducts and a top plane species in the plasma source:

```
add_reaction model=reaction_model  
    expression="SiCl<g> + I<t> = SiCl<v> + I<v>" name=r8
```

This reaction corresponds to an annihilation of the plasma radical $I<t>$, resulting in a decrease of the $I<t>$ concentration in the plasma bulk.

The following command adds a plasma enhancement reaction between gaseous surface reaction byproducts and a generic top plane species:

```
add_reaction model=reaction_model \  
    expression="SiCl<g> + <t> = 2Cl<g>" name=r9
```

This reaction represents a generic reaction between a surface reaction byproduct ($SiCl<g>$) and a generic plasma bulk particle (represented by the placeholder $<t>$) at the top plane, triggering the emission of two new plasma particles ($2Cl<g>$) and, therefore, leading to an enhancement of the plasma particle flux.

Example of BCA Reaction

Create a BCA reaction for Ar where Oxide sputters and is not tracked, Silicon sputters and is tracked, and CxFy sputters, becomes P, and is tracked:

```
add_reaction incoming_species=Ar \  
    target_species={Oxide Silicon CxFy} \  
    tracked_product_species={Silicon P} \  
    target_product_map={CxFy P}
```

Chapter 6: Input Commands

add_reaction_properties

add_reaction_properties

This command specifies the parameters of a reaction.

Syntax

For reflection reactions (see [add_reaction on page 182](#)):

```
add_reaction_properties (p=<n> | probability=<c>) reaction=<c> \
[<crystal_parameters>] [<energy_parameters>] \
[machine=<c>] [max_product_coverage=<n>] [reflection_exponent=<n>]
```

For sputtering reactions (see [add_reaction on page 182](#)):

```
add_reaction_properties (p=<n> | probability=<c>) reaction=<c> \
[<crystal_parameters>] [<energy_parameters>] [machine=<c>] \
[sputter_exponent=<n>] \
[(sputter_gamma=<n> [sputter_isotropic_ratio=<n>] \
[sputter_preferential_angle=<n>]) | sputter_type=<c>]
```

For adsorption or deposition reactions with surface diffusion (see [add_reaction on page 182](#) and [Diffusion on page 91](#)):

```
add_reaction_properties method=diffusion reaction=<c> \
(p=<n> | probability=<c>) reaction=<c> \
[alpha=<n>] \
[biased_random_walk=<c>] \
[<crystal_parameters>] [<energy_parameters>] \
[machine=<c>] [max_product_coverage=<n>] \
[num_diffusion_steps=<n>] \
[redistribution_factor=<n>]
```

For top plane reactions with gaseous reaction product (see [Example of Top Plane Reactions on page 187](#)):

```
add_reaction_properties reaction=<c> (p=<n> | probability=<c>) \
[machine=<c>] [product_distribution=<c>]
```

For other reactions:

```
add_reaction_properties (p=<n> | probability=<c>) reaction=<c> \
[<crystal_parameters>] [<energy_parameters>] \
[machine=<c>] [max_product_coverage=<n>]
```

Chapter 6: Input Commands

add_reaction_properties

Table 22 Parameters of add_reaction_properties command

Parameter	Description
activation_energy	Sets the value of the activation energy parameter E_a in Equation 79 . Type: Number Default: 0 Range: [0 , ∞ [Unit: eV
alpha	Controls the strength of the bias during a biased random walk. You can specify this parameter only for method=diffusion. Type: Number Default: 1 Range: [0 , ∞)
biased_random_walk	Specifies whether to execute the full random walk for the given number of diffusion steps (option last_step) or to terminate the random walk automatically when a suitable deposition site is found (option always). See Diffusion on page 91 for details. You can specify this parameter only for method=diffusion. Type: Character Default: always
<crystal_parameters>	See Crystal Parameters on page 195 . Type: Character Default: none
crystal_type	Sets the crystal type of the deposited crystalline material. This parameter can only be set for deposition reactions with product_morphology= crystalline. The only supported option is diamond. Type: Character Default: none
diamond_activation_energy_<hkl>	Sets the value of the activation energy parameter E_a in Equation 79 , when the solid reactant has a diamond crystal structure and its exposed surface is parallel to an (h k l) crystal plane, where <hkl> is 100 or 110 or 111. Type: Number Default: 0 Range: [0 , ∞ [Unit: eV

Chapter 6: Input Commands

add_reaction_properties

Table 22 Parameters of add_reaction_properties command (Continued)

Parameter	Description
diamond_energy_exponent_<hkl>	Sets the value of the exponent parameter m in Equation 80 , when the solid reactant has a diamond crystal structure and its exposed surface is parallel to an $(h k l)$ crystal plane, where <hkl> is 100 or 110 or 111. Type: Number Default: none Range:]0, ∞[
diamond_energy_reference_<hkl>	Sets the value of the parameter E_{ref} in Equation 80 , when the solid reactant has a diamond crystal structure and its exposed surface is parallel to an $(h k l)$ crystal plane, where <hkl> is 100 or 110 or 111. Type: Number Default: none Range:]0, ∞[Unit: eV
diamond_energy_threshold_<hkl>	Sets the value of the parameter E_{th} in Equation 80 , when the solid reactant has a diamond crystal structure and its exposed surface is parallel to an $(h k l)$ crystal plane, where <hkl> is 100 or 110 or 111. Type: Number Default: none Range:]0, ∞[Unit: eV
diamond_p_<hkl>	Sets the energy- and angle-independent value of the reaction probability to use when the solid reactant has a diamond crystal structure and its exposed surface is parallel to an $(h k l)$ crystal plane, where <hkl> is 100 or 110 or 111. Type: Number Default: none Range: [0, 1]
diamond_probability_<hkl>	Sets the name of the probability function defined with the <code>define_probability</code> command to use when the solid reactant has a diamond crystal structure and its exposed surface is parallel to an $(h k l)$ crystal plane, where <hkl> is 100 or 110 or 111. Type: Character Default: none

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add_reaction_properties

Table 22 Parameters of add_reaction_properties command (Continued)

Parameter	Description
<energy_parameters>	See Activation Energy on page 197 . Type: Character Default: none
energy_exponent	Sets the value of the exponent parameter m in Equation 80 . Type: Number Default: none Range:]0, ∞[
energy_reference	Sets the value of the parameter E_{ref} in Equation 80 . Type: Number Default: none Range:]0, ∞[Unit: eV
energy_threshold	Sets the value of the parameter E_{th} in Equation 80 . Type: Number Default: none Range:]0, ∞[Unit: eV
machine	Sets the name of the machine for which the reaction is configured. Type: Character Default: default_machine
max_product_coverage	Sets the maximum surface coverage of the reaction product with the <s> species-type modifier that allows the reaction to be executed. This parameter can be specified only if there is exactly one reaction product with the <s> species-type modifier. Type: Number Default: 1 Range: [0, 1]
method	If this parameter is set to diffusion, then it allows surface diffusion (see Diffusion on page 91). You can specify this parameter only for adsorption or deposition reactions. Type: Character Default: none

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add_reaction_properties

Table 22 Parameters of *add_reaction_properties* command (Continued)

Parameter	Description
num_diffusion_steps	Sets the number of steps of the random walk along the surface during deposition reactions. You can specify this parameter only for <code>method=diffusion</code> . Type: Number Default: 1 Range: [0, ∞)
p	Sets the energy- and angle-independent value of the reaction probability to use when the solid reactant is amorphous. Type: Number Default: none Range: [0, 1]
p_island_growth	Sets the probability that the gaseous reactant sticks to a preexisting island and takes over the crystal orientation of that island. Type: Number Default: none Range: [0, 1]
p_nucleation	Sets the probability that the gaseous reactant sticks to the surface and forms a new island with a random crystal orientation. Type: Number Default: none Range: [0, 1]
probability	Sets the name of the probability function defined with the <code>define_probability</code> command to use when the solid reactant is amorphous. Type: Character Default: none
product_distribution	Sets the name of the species distribution of the gaseous reaction product. Type: Character Default: The species distribution defined within the specified machine or, if the distribution of the species is undefined, an isotropic distribution (<code>exponent=1</code>)

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add_reaction_properties

Table 22 Parameters of *add_reaction_properties* command (Continued)

Parameter	Description
product_energy_factor	Sets the ratio between the energy of any reaction products with the <g>, <p>, or <r> species-type modifier and the energy of the gaseous reactant of the reaction being specified. Type: Number Default: 1 Range: [0, 1]
product_energy_max	Sets the maximum energy of the products with the <g>, <p>, or <r> species-type modifier of the reaction being specified, when they are assumed to have a uniform energy distribution. Type: Number Default: none Range:]0, ∞[Unit: eV
product_energy_min	Sets the minimum energy of the products with the <g>, <p>, or <r> species-type modifier of the reaction being specified, when they are assumed to have a uniform energy distribution. Type: Number Default: none Range:]0, ∞[Unit: eV
product_morphology	Sets the material type of the adsorbed or deposited species. Options are: <ul style="list-style-type: none">• amorphous• crystalline• same_as_surface_reactant Note: You can use the <code>crystalline</code> option only when modeling nucleation, that is, in combination with the parameters <code>p_nucleation</code> and <code>p_island_growth</code> (see Nucleation and Grain Growth on page 89). Type: Character Default: amorphous
reaction	Sets the name of the reaction to configure. Type: Character Default: none

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add_reaction_properties

Table 22 Parameters of `add_reaction_properties` command (Continued)

Parameter	Description
<code>redistribution_factor</code>	Sets the percentage of reactions for which the random walk is executed. You can specify this parameter only for <code>method=diffusion</code> . Type: Number Default: 1 Range: [0, 1]
<code>reflection_exponent</code>	Sets the exponent of the angular distribution $\cos^m\theta$ of the reflected species. If omitted, all particles are reflected along the direction specular to the incoming one with respect to the surface normal. Type: Default: Range: Unit:
<code>sputter_exponent</code>	Sets the exponent of the angular distribution $\cos^m\theta$ of the sputtered species. Type: Number Default: 1 Range: Energy-dependent expression, evaluating to]0, ∞[
<code>sputter_gamma</code>	Sets the value of γ in Equation 81 that controls the main direction of the emission of the sputtered material. You can use this parameter only if you do not use <code>sputter_type</code> . Note: Setting <code>sputter_gamma=0</code> and <code>sputter_exponent=1</code> is equivalent to <code>sputter_type=diffuse</code> . Type: Number Default: none Range:]-∞, ∞[
<code>sputter_isotropic_ratio</code>	Sets the ratio of particles that are sputtered isotropically for small incidence angles. It can be used only if you specify <code>sputter_preferential_angle</code> . Type: Number Default: 0 Range: Energy-dependent expression, evaluating to [0, 1]

Chapter 6: Input Commands

add_reaction_properties

Table 22 Parameters of add_reaction_properties command (Continued)

Parameter	Description
sputter_preferential_angle	Sets the preferential ejection angle θ_{pref} for sputtering under normal incidence angles (see Figure 23 on page 200). It can be used only if you specify sputter_gamma. Type: Number Default: 0 Range: Energy-dependent expression, evaluating to [0, 90] Unit: degree
sputter_type	Sets the sputter reemission type of the model. Options are: <ul style="list-style-type: none">• diffuse• reflective You can use this parameter only if you do not use sputter_gamma. If you do not use either sputter_gamma or sputter_type, then sputter_type=diffuse is used. Type: Character Default: none

Crystal Parameters

Note:

A single add_reaction_properties command specifies the reaction probabilities for both amorphous and crystalline or polycrystalline surface materials. For each surface material, you must always specify all probabilities since the structure can contain the same material both in amorphous and in crystalline or polycrystalline form. For example:

```
add_reaction_properties reaction=R p=1 \
    diamond_p_100=1 diamond_p_110=0.7 diamond_p_111=0.1
```

You must specify a collection of parameters for reactions involving crystalline materials:

- For etching or sputtering reactions on a crystalline surface (see [Etching and Sputtering Reactions on page 87](#)):

```
<crystal_parameters> =
  (<crystal_type>_p_<hkl>=<n> |
   <crystal_type>_probability_<hkl>=<c>) |
  [<crystal_type>_activation_energy_<hkl>=<n> |
   (<crystal_type>_energy_exponent_<hkl>=<n>
    <crystal_type>_energy_reference_<hkl>=<n>
    <crystal_type>_energy_threshold_<hkl>=<n>) ]
```

Chapter 6: Input Commands

add_reaction_properties

where:

- <crystal_type> stands for the crystal type of the surface (the only option is <crystal_type>=diamond)
- <hkl> stands for the Miller index ($h \ k \ l$) of the crystal plane on which this parameter is defined (for diamond, <hkl>=100, 110, or 111)

For example:

```
add_reaction_properties reaction=R p=1 \
    diamond_p_100=1 diamond_p_110=0.7 diamond_p_111=0.1
```

- For adsorption or deposition of material on a crystalline surface (see [Adsorption and Deposition Reactions on page 88](#)):

```
<crystal_parameters> =
  (<crystal_type>_p_<hkl>=<n> | 
   <crystal_type>_probability_<hkl>=<c>)
  [<crystal_type>_activation_energy_<hkl>=<n> |
   (<crystal_type>_energy_exponent_<hkl>=<n>
    <crystal_type>_energy_reference_<hkl>=<n>
    <crystal_type>_energy_threshold_<hkl>=<n>)]
  product_morphology=amorphous | same_as_surface_reactant
```

For example:

```
add_reaction_properties reaction=R p=1 \
    diamond_p_100=1 diamond_p_110=0.7 diamond_p_111=0.1 \
    product_morphology=amorphous
```

- For adsorption or deposition of crystalline material on an amorphous surface (see [Adsorption and Deposition Reactions on page 88](#)):

```
<crystal_parameters> =
  product_morphology=crystalline
  crystal_type=<c>
  p_island_growth=<n>
  p_nucleation=<n>
```

For example:

```
add_reaction_properties reaction=R p=1 \
    product_morphology=crystalline crystal_type=diamond \
    p_nucleation=1e-5 p_island_growth=1
```

Chapter 6: Input Commands

add_reaction_properties

Activation Energy

Note:

The following parameters are available only when the machine specified with the machine parameter is energy dependent:

```
<energy_parameters> =
  (activation_energy=<n> |
   energy_exponent=<n> energy_reference=<n> energy_threshold=<n>)
  (product_energy_factor=<n> |
   product_energy_max=<n> product_energy_min=<n>)
```

If you set the activation_energy parameter, the following energy-dependent reaction probability $p(E, \theta)$ is assumed for the reaction at hand:

$$p(E, \theta) = p(\theta) \exp\left(-\frac{E_a}{E}\right) \quad (79)$$

where:

- $p(\theta)$ denotes the probability specified with the `p` parameter or the angle-dependent probability function specified with the `probability` parameter.
- E_a denotes the value given to the `activation_energy` parameter. It is worth noting that, according to [Equation 79](#), the probability is not zero for energies smaller than the value of the `activation_energy` parameter, but it decays rapidly as the energy falls below such a value.

If the `probability` parameter specifies an energy-dependent probability, an error will be issued in this case.

When you specify the `energy_exponent`, `energy_reference`, and `energy_threshold` parameters, the following energy-dependent reaction probability $p(E, \theta)$ is assumed for the reaction at hand [\[2\]](#):

$$p(E, \theta) = p(\theta) \cdot \begin{cases} 0 & E \leq E_{\text{th}} \\ \frac{E^m - E_{\text{th}}^m}{E_{\text{ref}}^m - E_{\text{th}}^m} & E_{\text{th}} < E < E_{\text{ref}} \\ 1 & E \geq E_{\text{ref}} \end{cases} \quad (80)$$

In [Equation 80](#):

- $p(\theta)$ denotes the probability specified with the `p` parameter or the angle-dependent probability function specified with the `probability` parameter. It is the probability when the energy is greater than or equal to the value specified by the `energy_reference` parameter.
- m denotes the value given to the `energy_exponent` parameter.

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add_reaction_properties

- E_{ref} denotes the value (in electron volts) given to the `energy_reference` parameter.
- E_{th} denotes the value (in electron volts) given to the `energy_threshold` parameter.

If the `probability` parameter specifies an energy-dependent probability, then an error will be issued in this case.

The `product_energy_factor`, `product_energy_max`, and `product_energy_min` parameters can be specified only for reactions that have at least one product with the `<g>`, `<p>`, or `<r>` species-type modifier.

When parameter `product_energy_factor` is specified, the energy of the product having the `<g>`, `<p>`, or `<r>` species-type modifier will be proportional to the energy of the reactant with the `<g>` species-type modifier, and the proportionality constant will be the value of the `product_energy_factor` parameter.

When parameters `product_energy_max` and `product_energy_min` are specified, the energy of the product having the `<g>`, `<p>`, or `<r>` species-type modifier will be uniformly distributed over the energy window defined by the values of these two parameters.

The main direction in which sputtered particles are emitted can be controlled with the parameter `sputter_gamma`. It is used to specify the value of the parameter γ in the function $f(\theta, \gamma)$. This function is used to determine the angle between the surface normal and the symmetry axis of the sputter emission distribution.

The symmetry axis of the sputter emission distribution lies in the plane defined by the direction of the incoming particles and the surface normal. The angle between the symmetry axis of the sputter emission distribution and the surface normal is considered to be negative if the symmetry axis of the sputter emission distribution is on the same side of the surface normal as the direction of the incoming particles. Otherwise, it is considered to be positive.

$$f(\theta, \gamma) = \begin{cases} \gamma\theta & \text{for } 0 \leq |\gamma| \leq 1 \\ \text{sgn}(\gamma)\frac{\pi}{2}\left(1 - \left(1 - \frac{\theta}{\frac{\pi}{2}}\right)^{|\gamma|}\right) & \text{for } 1 \leq |\gamma| \end{cases} \quad (81)$$

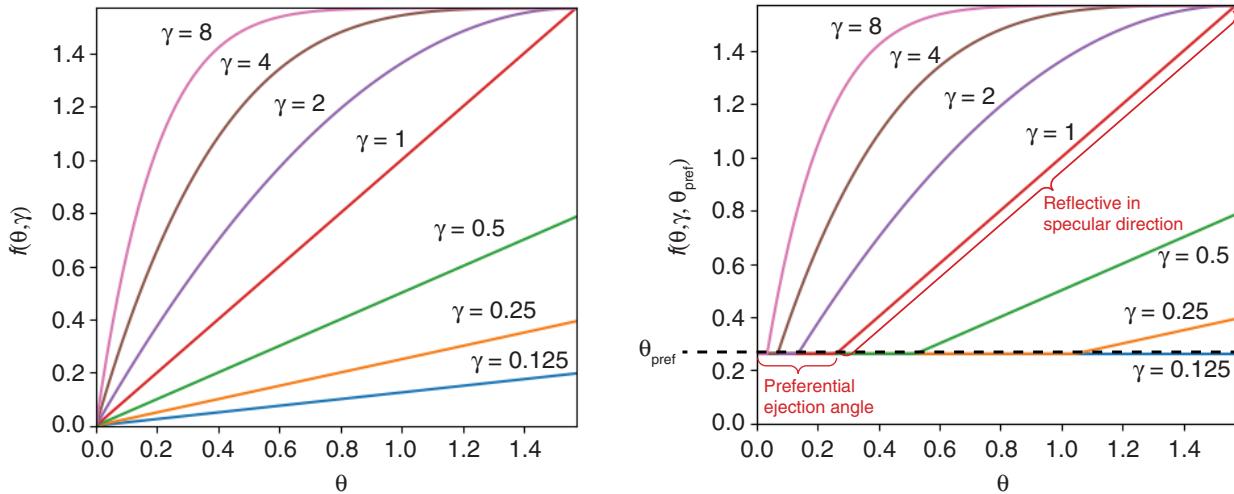
$$\text{where } \text{sgn}(x) = \begin{cases} +1 & \text{for } x > 0 \\ 0 & \text{for } x = 0 \\ -1 & \text{for } x < 0 \end{cases} .$$

[Figure 22 \(left\)](#) shows $f(\theta, \gamma)$ for different values of γ . The horizontal axis represents the angle θ between the surface normal and the incoming particle. The vertical axis represents the angle between the surface normal and the symmetry axis of the sputter emission distribution.

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`add_reaction_properties`

Figure 22 (Left) Function $f(\theta, \gamma)$ and (right) function $f(\theta, \gamma, \theta_{\text{pref}})$ for values of $\gamma = 0.125, 0.25, 0.5, 1, 2, 4$, and 8



For $\gamma = 0$, the symmetry axis of the sputter emission distribution is perpendicular to the surface. Therefore, `sputter_gamma=0` gives the same result as `sputter_type=diffuse`.

For $\gamma = 1$, the symmetry axis of the sputter emission distribution is the reflected direction of the incoming particle. Therefore, `sputter_gamma=1` gives the same result as `sputter_type=reflective`.

For $\gamma < 0$, the sputtered particles are not emitted forward as for positive values of γ , but back in the direction of the incoming particle.

You can also specify a preferential ejection angle for the emitted particle. This can be useful when modeling low-energetic sputtering processes, which are determined by under-cosine or heart-like sputter angle distributions. You define a preferential ejection angle for normally incident particles by using the `sputter_preferential_angle` parameter, which modifies the function $f(\theta, \gamma)$, as shown in Figure 22 (right).

For almost normally incident particles with small incidence angles, the sputtered particle is emitted with angle `sputter_preferential_angle` with a spread determined by `sputter_exponent`. For incident particles with oblique incidence angles, the outgoing particle is sputtered in the specular direction with a spread determined by `sputter_exponent`.

In addition, for normally incident particles, you can specify a ratio $p_0 \in [0, 1]$ of particles that will be sputtered isotropically (that is, with an angular spread $\cos\theta$) around the surface normal.

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add_reaction_properties

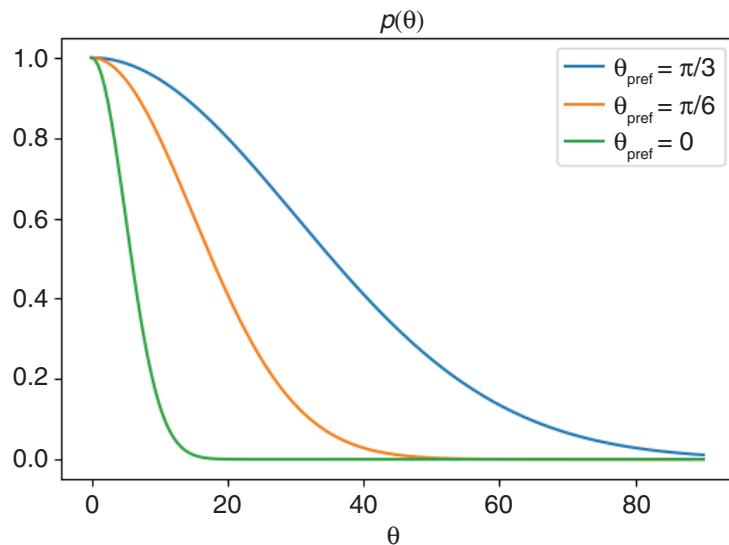
You can set this ratio by using the `sputter_isotropic_ratio` parameter. The ratio of isotropically sputtered particles depends on the incidence angle θ by the expression:

$$p(\theta) = p_0 \exp\left(-\frac{\theta^2}{2\sigma^2}\right) \quad (82)$$

where $\sigma = \frac{1}{2} \max(10^\circ, \theta_{\text{pref}})$ and θ_{pref} is the preferential ejection angle specified by the parameter `sputter_preferential_angle`.

For normal incidence angles ($\theta = 0$), the ratio equals `sputter_isotropic_ratio`. For oblique incidence angles ($\theta \rightarrow \pi/2$), the ratio decreases to zero.

Figure 23 Ratio of isotropically sputtered particles as a function of the incidence angle θ



Reaction Properties for Binary Collision Approximation Reactions

If an interaction is eligible for binary collision approximation (BCA) handling, to determine whether it is called depends on the reaction probability, which can be set in one of the following ways:

- `add_reaction_properties p=<n>`

In this case, there should not be a PMC reaction specified using the same `incoming_species`. If the BCA reaction is not called, then the default event for the source species is called (`default_event` parameter of the `define_species_properties` command)

- `add_reaction_properties probability=<c>`

In this case, there should not be a PMC reaction specified using the same `incoming_species`. If the BCA reaction is not called, then the default event for the

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add_reaction_properties

source species is called (default_event parameter of the define_species_properties command).

This specification is needed when a BCA reaction and one or more PMC reactions are defined using the same source species and have at least one target reactant in common. In this case, if no PMC reactions are called, then the specified BCA reaction is called.

Examples

```
# Reaction model definition
define_model name=m description=""

add_source_species model=m name=I
add_source_species model=m name=N

# Adsorption of species N on species Silicon
add_reaction model=m name=adsorption_reaction \
    expression="N<g> + Silicon<s> = SiliconN<s>"

# Reflection of species I by species Silicon
add_reaction model=m name=reflection_reaction \
    expression="I<g> + Photoresist<s> = I<r> + Photoresist<s>"

# Etching of species SiliconN by species I
add_reaction model=m name=ion_etch_reaction \
    expression="I<g> + SiliconN<s> = SiliconN<v>"

# Sputtering of species Silicon by species I
add_reaction model=m name=sputtering_reaction \
    expression="I<g> + Silicon<s> = Silicon<p>"
finalize_model model=m

# ...
# Define the yield function for sputtering of Silicon by species I
define_yield name=my_yield energy=0 species=I material=Silicon \
    theta_max=60 yield_max=1.4

# Define the probability function for reflection of species I
# from Photoresist
define_probability name=my_probability energy=0 mizuno_k=0.05

# Define a machine using the reaction model 'm'. Since the used
# model contains sputtering reactions, yield functions must be
# provided when defining the machine.
define_etch_machine model=m yield=my_yield ...

# Reactions 'adsorption_reaction' and 'ion_etch_reaction' are neither
# reflection nor sputtering reactions. Therefore, the parameter 'p'
# is used to set their angle-independent probabilities.
add_reaction_properties reaction=adsorption_reaction p=0.9
add_reaction_properties reaction=ion_etch_reaction p=0.7
```

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add_reaction_properties

```
# Reaction 'reflection_reaction' is a reflection reaction. Therefore,  
# it is possible to set parameter 'reflection_exponent' for it.  
# Moreover, the probability function defined with the  
# 'define_probability' command will be used as the reaction probability.  
add_reaction_properties reaction=reflection_reaction \  
    reflection_exponent=1000 probability=my_probability  
  
# Reaction 'sputtering_reaction' is a sputtering reaction. Therefore,  
# it is possible to set parameter 'sputter_exponent' for it. The  
# default value of parameter 'sputter_type' is used here.  
add_reaction_properties reaction=sputtering_reaction p=0.8 \  
    sputter_exponent=100
```

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add_source_species

add_source_species

This command adds a new source species to the specified reaction model.

Syntax

```
add_source_species model=<c> name=<c>
```

For binary collision approximation (BCA) reactions, which allow molecules to be used as source species but are split up into the atomic components when the molecule hits the surface:

```
add_source_species model=<c> name=<c> species=<l> stoichiometry=<l>
```

Table 23 Parameters of add_source_species command

Parameter	Description
model	<p>Sets the name of the model to which the source species is added.</p> <p>Note:</p> <p>This parameter must specify a reaction model, that is, the <code>type</code> parameter must <i>not</i> have been set in the <code>define_model</code> command for that model.</p> <p>Type: Character Default: none</p>
name	<p>Sets the name of the source species to add.</p> <p>Type: Character Default: none</p>
species	<p>Specifies a list of molecular incoming species in BCA reactions. This is a list of atoms that comprise the molecule.</p> <p>Type: List Default: none</p>
stoichiometry	<p>Specifies a list of the number of atoms corresponding to the <code>species</code> list, which comprise the molecule given by the <code>name</code> parameter. The length of the <code>stoichiometry</code> list must equal the length of the <code>species</code> list.</p> <p>Type: List Default: none</p>

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add_source_species

Examples

For a BCA reaction, C₄F₈ can be handled as four C and eight F atoms when this molecule hits the surface and would be specified with:

```
add_source_species model=bca_model name=C4F8 \
    species={Carbon Fluorine} stoichiometry={ 4 8 }
```

Then, it can be used in add_reaction and define_species_distribution commands:

```
add_reaction model=bca_model incoming_species=C4F8 \
    target_species=...
```

```
define_species_distribution name=sdd species=C4F8 flux=...
```

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add_species

add_species

This command adds a new plasma species to a specified plasma model.

Note:

If you specify an `add_species` command with the name of a plasma species that already exists, then this command is ignored.

Syntax

```
add_species charge=<n> mass=<n> name=<c> plasma_model=<c>
```

Table 24 Parameters of add_species command

Parameter	Description
charge	Sets the charge of the species in units of the unit charge e. Only single-charged species are allowed. Type: Number Default: none Range: {-1, 0, +1} Unit: e
mass	Sets the mass of the species. Type: Number Default: none Range:]0, +∞[Unit: amu
name	Sets the name of the plasma species. This name is used to refer to the species in other commands (for example, in plasma bulk reaction expressions, or when defining species-dependent plasma parameters in the <code>define_reactor</code> command). See define_reactor on page 301 . Note: Plasma species names must not contain spaces and must not begin with a number. The name <code>e-</code> is predefined for electrons and cannot be used. Type: Character Default: none
plasma_model	Sets the name of the plasma model to which the species is added. This model must be already defined by using define_plasma_model on page 298 . Type: Character Default: none

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add_volumetric_source_species

Examples

```
add_species name=Ar+ plasma_model=M mass=40<amu> charge=+1
```

add_volumetric_source_species

This command adds a new volumetric source species to a reaction model.

Syntax

```
add_volumetric_source_species model=<c> name=<c>
```

Table 25 Parameters of *add_volumetric_source_species* command

Parameter	Description
model	<p>Sets the name of the model to which the volumetric source species is added.</p> <p>Note: This parameter must specify a reaction model, that is, the <code>type</code> parameter must not have been set in the <code>define_model</code> command for that model (see define_model on page 289).</p> <p>Type: Character Default: none</p>
name	<p>Sets the name of the volumetric source species to add.</p> <p>No <code>add_volumetric_source_species</code> commands must have been specified for the same model with the same <code>name</code> value.</p> <p>Type: Character Default: none</p>

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define_boundary_conditions

define_boundary_conditions

This command defines the boundary conditions to apply when using a structure in a simulation.

Syntax

```
define_boundary_conditions [structure=<c>] [x=<c>] [y=<c>] \
    [xmin=<c>] [xmax=<c>] [ymin=<c>] [ymax=<c>]
```

Table 26 Parameters of *define_boundary_conditions* command

Parameter	Description
structure	Sets the name of the structure for which boundary conditions must be defined. Type: Character Default: default_structure
x	Sets the boundary conditions for both planes $x = x_{\text{min}}$ and $x = x_{\text{max}}$, where x_{min} and x_{max} are the minimum and the maximum x-value in the simulation domain, respectively. Options are: <ul style="list-style-type: none">• none• periodic• reflective Type: Character Default: none
xmax	Sets the boundary conditions for the plane $x = x_{\text{max}}$, where x_{max} is the maximum x-value in the simulation domain. Options are: <ul style="list-style-type: none">• none• reflective Type: Character Default: reflective
xmin	Sets the boundary conditions for the plane $x = x_{\text{min}}$, where x_{min} is the minimum x-value in the simulation domain. Options are: <ul style="list-style-type: none">• none• reflective Type: Character Default: reflective

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define_boundary_conditions

Table 26 Parameters of *define_boundary_conditions* command (Continued)

Parameter	Description
y	Sets the boundary conditions for both planes $y = y_{\min}$ and $y = y_{\max}$, where y_{\min} and y_{\max} are the minimum and the maximum y -value in the simulation domain, respectively. Options are: <ul style="list-style-type: none">• none• periodic• reflective Type: Character Default: none
ymax	Sets the boundary conditions for the plane $y = y_{\max}$, where y_{\max} is the maximum y -value in the simulation domain. Options are: <ul style="list-style-type: none">• none• reflective Type: Character Default: reflective
ymin	Sets the boundary conditions for the plane $y = y_{\min}$, where y_{\min} is the minimum y -value in the simulation domain. Options are: <ul style="list-style-type: none">• none• reflective Type: Character Default: reflective

Limitations

The following limitations or conditions apply:

- When using a level set-based model, the boundary conditions are set automatically to `none` in the planes in which a user-defined tilt breaks the symmetry. When using the PMC method, periodic boundary conditions are applied automatically to the planes in which a user-defined tilt breaks the symmetry (see [Structure Tilt on page 37](#) and [Boundary Conditions on page 38](#)).
- The structure referred to by the `structure` parameter must be already defined before the `define_boundary_conditions` command is called.
- The `define_boundary_conditions` command affects not only flux computation, but also surface evolution. Therefore, this command is also relevant for non-flux models.

Chapter 6: Input Commands

define_boundary_conditions

- The `define_boundary_conditions` command has no effect on the built-in deposition model `crystal` and the built-in etch model `crystal`. Boundary conditions are always reflective when using those models.
- The boundary conditions specified by the command `define_boundary_conditions` have no effect on the indirect flux computations for 2D structures.
- Only `reflective` boundary conditions are supported when using the `electrodeposition`, `spin_on`, or `wet` built-in deposition model.
- When using RFM models that use the `pad_pressure()` RFM function, boundary conditions specified by the command `define_boundary_conditions` are ignored and periodic boundary conditions are always applied.
- When using the PMC method, boundary conditions of type `none` are not available.
- You can specify periodic boundary conditions only for the PMC method.
- The `x` parameter cannot be simultaneously specified with either the `xmin` parameter or the `xmax` parameter. The `y` parameter cannot be simultaneously specified with either the `ymin` parameter or the `ymax` parameter.

Examples

This command sets the boundary conditions on the two x-bounding planes of the structure called `default_structure` and uses the default ones on the two y-bounding planes. The plane with the minimum `x` will be considered as a reflective boundary; while in the plane of maximum `x`, the boundary condition type `none` will be applied:

```
define_boundary_conditions xmin=reflective xmax=none
```

Chapter 6: Input Commands

define_bulk_solver

define_bulk_solver

This optional command defines the numeric parameters of the ordinary differential equation (ODE) solver used for a plasma bulk model.

Syntax

```
define_bulk_solver bulk_model_type=<c> name=<c> \
    [abs_error=<n>] [convergence_check_num_samples=<n>] \
    [convergence_check_step=<n>] [max_num_steps=<n>] \
    [max_time=<n>] [rel_error=<n>] \
    [stationary_state_tolerance=<n>] [step_size=<n>] \
    [time_average_solution=<b>]
```

Table 27 Parameters of *define_bulk_solver* command

Parameter	Description
abs_error	Sets the absolute error used for adaptive step size control. Type: Number Default: 10^{-8} Range: $[0, \infty[$
bulk_model_type	Sets the type of the bulk model to solve. The only option is <code>global</code> . Type: Character Default: none Range: Unit:
convergence_check_num_samples	Sets the minimum number of samples to use when computing the convergence residual. Type: Number Default: 10^4 Range: $[1, \infty[$
convergence_check_step	Sets the interval at which convergence to the stationary state is computed. Type: Number Default: 10 Range: $[1, \infty[$
max_num_steps	Sets the maximum number of steps until convergence to the stationary state. Type: Number Default: 10^{10} Range: $[1, \infty[$

Chapter 6: Input Commands

define_bulk_solver

Table 27 Parameters of *define_bulk_solver* command (Continued)

Parameter	Description
max_time	Sets the maximum time to which the model is integrated to reach the stationary state. Type: Number Default: ∞ Range:]0, ∞ [Unit: s
name	Sets the name of the solver. This name is used to reference the solver in other commands, such as <code>solve_reactor</code> (see solve_reactor on page 548). Type: Character Default: none
rel_error	Sets the relative error used for the adaptive step size control. Type: Number Default: 10^{-8} Range:]0, ∞ [
stationary_state_tolerance	Sets the threshold for convergence to the stationary state. Type: Number Default: 10^{-4} Range:]0, ∞ [
step_size	Sets the initial step size, which might change due to the adaptive step size control. Type: Number Default: 10^{-6} Range:]0, ∞ [Unit: s
time_average_solution	When simulating pulsed power waveforms, this parameter specifies whether the bulk solution, consisting of periodic waveforms, should be averaged in time. Type: Boolean Default: False

Chapter 6: Input Commands

define_bulk_solver

Note:

For the define_bulk_solver command:

- Convergence speed is mainly influenced by the parameters convergence_check_step and stationary_state_tolerance.
- If the iterative bulk solver exceeds the maximum number of steps (max_num_steps) or the maximum simulation time (max_time), the solver returns an error stating that the plasma bulk model did not succeed.
- A default bulk solver, default_global_bulk_solver, is implicitly defined and can be referenced by other commands, such as solve_reactor (see [solve_reactor on page 548](#)). The implicit definition of this solver is equivalent to:

```
define_bulk_solver name=default_global_bulk_solver \
bulk_model_type=global
```

Examples

```
define_bulk_solver name=s1 bulk_model_type=global \
abs_error=1e-8 rel_error=1e-8 \
max_num_steps=1000000 max_time=1000<s> step_size=1e-6<s> \
stationary_state_tolerance=1e-4
```

Chapter 6: Input Commands

define_charging_model

define_charging_model

This command defines a charging model for charge-up simulations with a PMC model. You can define the model parameters including the charge-up factor, the boundary conditions for the electric field, and the electron angle distribution.

Syntax

```
define_charging_model name=<c> \
    (charge_dose=<n> | charging_factor=<n>) \
    [bottom_bc=<c>] \
    [bottom_electric_field=<n> | bottom_potential=<n>] \
    [charge_scaling=<n> | num_samples_per_cell=<n>] \
    [electric_contacts=<l>] \
    [electron_exponents=<l> electron_fluxes=<l>] \
    [enforce_charge_neutrality=<b>] \
    [top_bc=<c>] [top_electric_field=<n> | top_potential=<n>]
```

Table 28 Parameters of *define_charging_model* command

Parameter	Description
bottom_bc	Sets the boundary condition of the electric solver at the bottom of the simulation domain. Options are: <ul style="list-style-type: none">• dirichlet• floating• neumann Type: Character Default: dirichlet
bottom_electric_field	Sets the normal electric field at the lower Neumann boundary. You can specify this parameter only if <code>top_bc=neumann</code> . Type: Number Default: 0 Range: $(-\infty, \infty)$ Unit: V/m
bottom_potential	Sets the potential applied at the Dirichlet boundary at the bottom of the simulation domain. You can specify this parameter only if <code>bottom_bc=dirichlet</code> . Type: Number Default: 0 Range: $(-\infty, \infty)$ Unit: V

Chapter 6: Input Commands

define_charging_model

Table 28 Parameters of *define_charging_model* command (Continued)

Parameter	Description
charge_dose	<p>Sets the dose of charges sent to the structure, measured in the number of charges through a flat xy cross-section plane at a constant height z.</p> <p>You can specify either <code>charge_dose</code> or <code>charging_factor</code>.</p> <p>Type: Number Default: none Range: $[0, \infty)$ Unit: m^{-2}</p>
charge_scaling	<p>Sets a scaling factor used to reduce or enhance the charges deposited in the structure.</p> <p>This parameter controls the statistics and smoothness of the charge distribution on the surface during the charging phase. (It does not affect the physical total charge.)</p> <p>You can specify either <code>charge_scaling</code> or <code>num_samples_per_cell</code>.</p> <p>Type: Number Default: none Range: $[0, \infty)$</p>
charging_factor	<p>Sets the factor to control the strength of the charging effect. The factor determines the charge dose sent to the structure during the charging simulation.</p> <p>If <code>charging_factor=1</code>, then the reference charge dose is $10^{17} \text{ m}^{-2} = 0.1 \text{ nm}^{-2}$.</p> <p>You can specify either <code>charge_dose</code> or <code>charging_factor</code>.</p> <p>Type: Number Default: none Range: $[0, \infty)$</p>
electric_contacts	<p>Specifies a list of names referring to electric contacts defined in the <code>define_electric_contact</code> command.</p> <p>Type: List Default: none</p>
electron_exponents	<p>Specifies the exponent parameters $\{m_i\}$ of the angle distribution for the electrons.</p> <p>See parameter <code>electron_fluxes</code> for details.</p> <p>Type: List Default: none Range: $[1, \infty[$ for each entry in the list</p>

Chapter 6: Input Commands

define_charging_model

Table 28 Parameters of `define_charging_model` command (Continued)

Parameter	Description
electron_fluxes	<p>Sets the flux values $\{\Gamma_i\}$ of the angle distribution for the electrons, given by:</p> $f(\theta) = \frac{1}{2\pi} \sum_i \Gamma_i \cdot (m_i + 1) \cdot \cos^{m_i}(\theta)$ <p>where parameters m_i are specified by parameter <code>electron_exponents</code>.</p> <p>If not specified, then an isotropic distribution is used:</p> $f(\theta) = \frac{\Gamma_e}{\pi} \cos(\theta)$ <p>Note: The total electron flux $\Gamma_e = \sum_i \Gamma_i$ is rescaled to match the total ion flux to satisfy the charge neutrality condition. To switch off rescaling, set <code>enforce_charge_neutrality=false</code>.</p> <p>Type: List Default: none Range: $[0, \infty]$ for each value in the list Unit: mol/m²/s</p>
enforce_charge_neutrality	<p>Specifies whether to rescale the total electron flux such that it equals the total ion flux (to satisfy the charge neutrality condition).</p> <p>Type: Boolean Default: true</p>
name	<p>Sets the name of the charging model object. This name is referenced in the <code>define_etch_machine</code> command (see define_etch_machine on page 242).</p> <p>Type: Character Default: none</p>
num_samples_per_cell	<p>Sets the number of charges per source area cell, sent to the structure during the charging simulation.</p> <p>This parameter controls the statistics and smoothness of the charge distribution on the surface during the charging phase. (It does not affect the physical total charge.)</p> <p>You can specify either <code>charge_scaling</code> or <code>num_samples_per_cell</code>.</p> <p>Type: Number Default: 100 Range: $[0, \infty)$</p>

Chapter 6: Input Commands

define_charging_model

Table 28 Parameters of *define_charging_model* command (Continued)

Parameter	Description
top_bc	Sets the boundary condition of the electric solver at the top of the simulation domain. Options are: <ul style="list-style-type: none">• dirichlet• floating• neumann Type: Character Default: neumann
top_electric_field	Sets the normal electric field at the upper Neumann boundary. You can specify this parameter only if <code>top_bc=neumann</code> . Type: Number Default: 0 Range: $(-\infty, \infty)$ Unit: V/m
top_potential	Sets the potential applied at the Dirichlet boundary at the top of the simulation domain. You can specify this parameter only if <code>top_bc=dirichlet</code> . Type: Number Default: 0 Range: $(-\infty, \infty)$ Unit: V

Examples

```
define_charging_model name=cm charging_factor=1 top_electric_field=-1e6
```

Chapter 6: Input Commands

define_damage

define_damage

This command defines the parameters of the damage model (see [Analytic Damage Modeling on page 94](#)).

Syntax

```
define_damage energy=<v> material=<c> name=<c> projected_range=<v> \
sigma=<v> sigma_lateral=<v> species=<c> total_damage=<n> type=<c> \
[max_depth=<n>] [max_lateral=<n>]
```

Table 29 Parameters of *define_damage* command

Parameter	Description
energy	Sets the energies corresponding to the energy-dependent parameters <code>projected_range</code> , <code>sigma</code> , and <code>sigma_lateral</code> . All four parameters are vectors of the same length. Type: Vector Default: none Unit: eV
material	Sets the material for which damage should accumulate. The <code>define_damage</code> command should be called multiple times for every combination of material and species that add to the accumulated damage. Type: Character Default: none
max_depth	For performance reasons, damage is computed only to <code>max_depth</code> from the point where the specified species impacts the surface. Type: Number Default: $R_p + 3.0 \times \text{sigma}$ Unit: μm
max_lateral	For performance reasons, damage is computed only to <code>max_lateral</code> from the point where the specified species impacts the surface. Type: Number Default: $3.0 \times \text{sigma}_\text{lateral}$ Unit: μm
name	Sets the name of the damage parameter set. Type: Character Default: none

Chapter 6: Input Commands

define_damage

Table 29 Parameters of define_damage command (Continued)

Parameter	Description
projected_range	Sets R_p , the peak of the profile. Type: Vector Default: none Unit: μm
sigma	Sets σ , the spread of the profile in the primary direction. Type: Vector Default: none Unit: μm
sigma_lateral	Sets σ_l , the spread of the profile in the lateral direction. Type: Vector Default: none Unit: μm
species	Sets the species for which damage should accumulate. The define_damage command is called multiple times for each species and material specified. Type: Character Default: none
total_damage	Specifies the damage scale. Type: Number Default: none Unit: μm^{-2}
type	Sets the type of damage calculation to use. Options are: <ul style="list-style-type: none">• analytic_expression• hobler Type: Character Default: none

Description

The projected_range, sigma, and sigma_lateral parameters are specified as a piecewise linear function of energy, specifying a set of equal-length double arrays along with a double array of corresponding energies. For example:

```
define_damage <other required parameters> \
    energy = { 110.0<eV> 220.0<eV> 330.0<eV> } \
    projected_range = { 4.0<nm> 5.0<nm> 6.0<nm> } \
```

Chapter 6: Input Commands

define_damage

```
sigma = { 0.70<nm> 0.80<nm> 0.90<nm> } \
sigma_lateral = { 0.7<nm> 0.75<nm> 0.8<nm> }
```

where the projected range is 5 nm for energy 220 eV. Similarly, `sigma`=0.7 nm for 110 eV and 0.9 nm for 330 eV.

In addition, the parameters `max_depth` and `max_lateral` can be specified to balance accuracy with performance. Due to the large number of ion impacts in a typical simulation, the damage calculation can be computationally expensive. These parameters limit the domain considered for damage accumulation and are typically set to a small multiple (for example, 3) of `sigma` and `sigma_lateral`, respectively.

Examples

```
define_damage name=mydamage type=hobler species=N material=Nitride \
    total_damage=1.0 max_depth=5<nm> max_lateral=1.5<nm> \
    energy = { 110.0<eV> 220.0<eV> 330.0<eV> } \
    projected_range = { 2.0<nm> 2.25<nm> 2.5<nm> } \
    sigma = { 0.20<nm> 0.25<nm> 0.3<nm> } \
    sigma_lateral = { 0.2<nm> 0.25<nm> 0.3<nm> }

define_damage name=mydamage type=hobler species=N material=resist \
    total_damage=2.0 max_depth=4.5<nm> max_lateral=1.25<nm> \
    energy = { 100<eV> 200<eV> 300<eV> } \
    projected_range = { 1.75<nm> 2.0<nm> 2.25<nm> } \
    sigma = { 0.175<nm> 0.2<nm> 0.225<nm> } \
    sigma_lateral = { 0.175<nm> 0.2<nm> 0.225<nm> }
```

Chapter 6: Input Commands

```
define_deposit_machine
```

define_deposit_machine

This command defines a new machine for a deposition process. A deposition model can be specified with the parameter `model`.

Syntax

Atomic layer deposition:

```
define_deposit_machine anisotropy=<n> conformality=<n> \
cycle_duration=<n> (exponent=<n> | iad=<c>) \
growth_per_cycle=<n> material=<c> model=ald sticking=<n> \
[nad=<c> | neutral_exponent=<n>] [name=<c>] [rotation=<n>] [tilt=<n>]
```

Crystal orientation-dependent deposition:

```
define_deposit_machine material=<c> model=crystal rate_100=<n> \
rate_110=<n> rate_111=<n> \
[name=<c>] [selective_materials=<l>]
```

Electrodeposition:

```
define_deposit_machine acc_adsorption_rate=<n> \
acc_bulk_concentration=<n> bulk_distance=<n> \
depo_bulk_concentration=<n> exchange_current_density=<n> \
exchange_current_density_acc=<n> exchange_current_density_inh=<n> \
inh_adsorption_rate=<n> inh_bulk_concentration=<n> \
inh_diffusivity=<n> inh_displacement_rate=<n> \
material=<c> model=electrodeposition overpotential=<n> \
temperature=<n> \
[acc_alpha=<n>] [acc_diffusivity=<n>] \
[acc_saturation_surface_concentration=<n>] [alpha=<n>] \
[curvature_scaling=<n>] [depo_diffusivity=<n>] \
[depo_molar_volume=<n>] [depo_reference_concentration=<n>] \
[duty_cycle=<n>] [inh_alpha=<n>] \
[inh_saturation_surface_concentration=<n>] [name=<c>] \
[overpotential_off=<n>] [z=<n>] [z_alpha=<n>]
```

Electroplating deposition:

```
define_deposit_machine delta=<n> material=<c> model=electroplating \
rate=<n> [name=<c>]
```

High-density plasma deposition:

```
define_deposit_machine anisotropy=<n> (exponent=<n> | iad=<c>) \
material=<c> model=hdp rate=<n> redeposition=<n> \
s1=<n> s2=<n> sputter_rate=<n> sticking=<n> \
[nad=<c> | neutral_exponent=<n>] [name=<c>] [rotation=<n>] [tilt=<n>]
```

Chapter 6: Input Commands

```
define_deposit_machine
```

High-density plasma 2 deposition:

```
define_deposit_machine anisotropy=<n> (exponent=<n> | iad=<c>) \
material=<c> model=hdp2 \
rate=<n> reflection=<n> redeposition=<n> s1=<n> s2=<n> \
sputter_exponent=<n> sputter_rate=<n> sputter_type=<c> sticking=<n> \
[nad=<c> | neutral_exponent=<n>] [name=<c>] [rotation=<n>] [tilt=<n>]
```

Low-pressure chemical vapor deposition:

```
define_deposit_machine material=<c> model=lpcvd rate=<n> sticking=<n> \
[nad=<c> | neutral_exponent=<n>] [name=<c>] [rotation=<n>] [tilt=<n>]
```

Plasma-enhanced chemical vapor deposition:

```
define_deposit_machine anisotropy=<n> (exponent=<n> | iad=<c>) \
material=<c> model=pecvd rate=<n> sticking=<n> \
[nad=<c> | neutral_exponent=<n>] [name=<c>] [rotation=<n>] [tilt=<n>]
```

Physical vapor deposition:

```
define_deposit_machine (exponent=<n> | iad=<c>) material=<c> model=pvd \
rate=<n> [name=<c>] [rotation=<n>] [tilt=<n>]
```

Simple deposition:

```
define_deposit_machine anisotropy=<n> curvature=<n> material=<c> \
model=simple rate=<n> [name=<c>] [rotation=<n>] [tilt=<n>]
```

Spin-on-glass deposition:

```
define_deposit_machine angular_position=<n> angular_velocity=<n> \
density=<n> evaporation_rate=<n> initial_thickness=<n> \
material=<c> model=spin_on \
radial_distance=<n> surface_tension=<n> viscosity=<n> [name=<c>]
```

RFM model:

```
define_deposit_machine material=<c> model=<c> [iad=<c>] \
[maximum_error=<n>] [nad=<c>] [name=<c>] [reflection=<c>] \
[rotation=<n> | <c>] [tilt=<n>] [yield=<c>] ...
```

Chapter 6: Input Commands

define_deposit_machine

Table 30 Parameters of *define_deposit_machine* command

Parameter	Description
acc_adsorption_rate	Sets the rate constant of the accelerator adsorption reaction. Type: Number Default: none Range:]0, ∞[Unit: μm/min
acc_alpha	Sets the transfer coefficient for a surface fully covered by accelerators. Type: Number Default: 0.4 (from [3]) Range:]0, 1]
acc_bulk_concentration	Sets the bulk concentration of accelerators. Type: Number Default: none Range:]0, ∞[Unit: mol/cm ³
acc_diffusivity	Sets the diffusivity of accelerators. If this parameter is omitted, the concentration of accelerators will be assumed to equal the value provided by the parameter acc_bulk_concentration everywhere. Type: Number Default: none Range:]0, ∞[Unit: cm ² /s
acc_saturation_surface_concentration	Sets the accelerator surface concentration of a surface fully covered by accelerators. Type: Number Default: 8e-10 (from [3]) Range:]0, ∞[Unit: mol/cm ²
alpha	Sets the transfer coefficient for a clean surface, that is, for a surface where no additives are adsorbed. Type: Number Default: 0.5 (from [3]) Range:]0, 1]

Chapter 6: Input Commands

define_deposit_machine

Table 30 Parameters of *define_deposit_machine* command (Continued)

Parameter	Description
angular_position	Sets the angle between the plane that contains the yz plane of the wafer coordinate system and the plane that contains the z-axis of the wafer coordinate system and the center of the structure on which the process occurs. Type: Number Default: none Range: [-180, 180] Unit: degree
angular_velocity	Sets the angular velocity of the wafer. Type: Number Default: none Range: [0, ∞[Unit: rpm
anisotropy	Sets the anisotropy coefficient. Type: Number Default: none Range: [0, 1]
bulk_distance	Sets the distance from the topmost point of the exposed surface of the plane where the species concentrations are assumed to equal their bulk values. Type: Number Default: none Range:]0, ∞[Unit: μm
conformality	Sets the conformality parameter for the atomic layer deposition (ALD) process. Type: Number Default: none Range:]0, ∞[
curvature	Sets the curvature coefficient. Type: Number Default: none Range: [0, 0.1] Unit: μm

Chapter 6: Input Commands

define_deposit_machine

Table 30 Parameters of *define_deposit_machine* command (Continued)

Parameter	Description
curvature_scaling	Sets the factor by which the surface mean curvature is scaled to update the additive surface coverage. Type: Number Default: 1 Range:]0, ∞[
cycle_duration	Sets the duration of one deposition cycle. Type: Number Default: none Range:]0, ∞[Unit: s
delta	Sets the gradient of the accelerator surface concentration for the electrodeposition model. Type: Number Default: none Range:]0, ∞[Unit: μm^{-1}
density	Sets the density of the film to be deposited. Type: Number Default: none Range:]0, ∞[Unit: g/cm
depo_bulk_concentration	Sets the bulk concentration of the deposited material. Type: Number Default: none Range:]0, ∞[Unit: mol/cm ³
depo_diffusivity	Sets the diffusivity of the deposited material. If this parameter is omitted, the concentration of the material being deposited is assumed to equal its bulk value. Type: Number Default: none Range:]0, ∞[Unit: cm ² /s

Chapter 6: Input Commands

define_deposit_machine

Table 30 Parameters of define_deposit_machine command (Continued)

Parameter	Description
depo_molar_volume	Sets the molar volume of the deposited material. Type: Number Default: 7.1e-6 (from [4]) Range: [0, ∞[Unit: m ³ /mol
depo_reference_concentration	Sets the concentration at which exchange current densities are measured. If this parameter is omitted, the value of the parameter depo_bulk_concentration is assumed as the reference concentration. Type: Number Default: none Range:]0, ∞[Unit: mol/cm ³
duty_cycle	Sets the duty cycle of the overpotential, that is, a fraction of a pulse period. The overpotential takes the value given by the overpotential parameter. In the remaining time of a pulse period, the overpotential is assumed to equal the value given by the overpotential_off parameter. Type: Number Default: 1 Range: (0, 1]
evaporation_rate	Sets the evaporation rate of the film to be deposited. Type: Number Default: none Range: [0, ∞[Unit: μm min ⁻¹
exchange_current_density	Sets the exchange current density on a free surface, measured at the reference concentration set by the parameter depo_reference_concentration. Type: Number Default: none Range: [0, ∞[Unit: mA/cm ²

Chapter 6: Input Commands

define_deposit_machine

Table 30 Parameters of define_deposit_machine command (Continued)

Parameter	Description
exchange_current_density_acc	Sets the exchange current density on a surface fully covered by accelerators, measured at the reference concentration set by the parameter depo_reference_concentration. Type: Number Default: none Range: $[0, \infty[$ Unit: mA/cm ²
exchange_current_density_inh	Sets the exchange current density on a surface fully covered by inhibitors, measured at the reference concentration set by the parameter depo_reference_concentration. Type: Number Default: none Range: $[0, \infty[$ Unit: mA/cm ²
exponent	Sets the exponent used to characterize the ion angular distribution $\cos^m\theta$. Type: Number Default: none Range: $[1, \infty[$
growth_per_cycle	Sets the growth per cycle. Type: Number Default: none Range: $[0, \infty[$ Unit: μm
iad	Sets the name of the IAD to be used. Type: Character Default: none
inh_adsorption_rate	Sets the rate constant of the inhibitor adsorption reaction. Type: Number Default: none Range: $[0, \infty[$ Unit: μm/min

Chapter 6: Input Commands

define_deposit_machine

Table 30 Parameters of define_deposit_machine command (Continued)

Parameter	Description
inh_alpha	Sets the transfer coefficient for a surface fully covered by inhibitors. Type: Number Default: 0.5 (from [3]) Range: [0, 1]
inh_bulk_concentration	Sets the bulk concentration of inhibitors. Type: Number Default: none Range:]0, ∞[Unit: mol/cm ³
inh_diffusivity	Sets the diffusivity of inhibitors. Type: Number Default: none Range:]0, ∞[Unit: cm ² /s
inh_displacement_rate	Sets the rate constant of the reaction by which inhibitors are displaced by accelerators. Type: Number Default: none Range:]0, ∞[Unit: μm/min
inh_saturation_surface_concentration	Sets the inhibitor surface concentration of a surface fully covered by inhibitors. Type: Number Default: 6e-11 (from [3]) Range:]0, ∞[Unit: mol/cm ²
initial_thickness	Sets the thickness of the film over the substrate when the spin-on simulation starts. Type: Number Default: none Range:]0, ∞[Unit: μm

Chapter 6: Input Commands

define_deposit_machine

Table 30 Parameters of *define_deposit_machine* command (Continued)

Parameter	Description
material	Sets the material to be deposited. Type: Character Default: none
maximum_error	Sets the maximum tolerated equivalence error for all species of the model. This parameter can be used only if rotation=continuous. See Continuously Rotating and Tilted Structure Modeling on page 57 . Type: Number Default: 0.5 Range: [0, 0.5]
model	Sets the model used to represent the physical machine. Type: Character Default: none
nad	Sets the name of the neutral angular distribution (NAD) to be used. Type: Character Default: none
name	Sets the name of the machine. Type: Character Default: default_machine
neutral_exponent	Sets the exponent used to characterize the NAD $\cos^m\theta$. Type: Number Default: 1 Range: [1, ∞ [
overpotential	Sets the overpotential of the electroplating cell during the on-cycle of the overpotential pulse. Type: Number Default: none Range:] $-\infty$, 0] Unit: V

Chapter 6: Input Commands

define_deposit_machine

Table 30 Parameters of *define_deposit_machine* command (Continued)

Parameter	Description
overpotential_off	Sets the overpotential of the electroplating cell during the off-cycle of the overpotential pulse. This parameter can be specified only when <code>duty_cycle</code> is less than 1. Type: Number Default: 0 Range:]-∞, 0] Unit: V
radial_distance	Sets the distance of the center of the feature from the axis of rotation of the wafer. Type: Number Default: none Range: [0, ∞[Unit: μm
rate	Sets the deposition rate. Type: Number Default: none Unit: μm min ⁻¹
rate_100	Sets the deposition rate for the <100> direction. Type: Number Default: none Range: [0, ∞[Unit: μm min ⁻¹
rate_110	Sets the deposition rate for the <110> direction. Type: Number Default: none Range: [0, ∞[Unit: μm min ⁻¹
rate_111	Sets the deposition rate for the <111> direction. Type: Number Default: none Range: [0, ∞[Unit: μm min ⁻¹

Chapter 6: Input Commands

define_deposit_machine

Table 30 Parameters of define_deposit_machine command (Continued)

Parameter	Description
redeposition	Sets the ratio of the amount of material redeposited to the amount of material sputtered from the surface. Type: Number Default: none Range: [0, 1]
reflection	For built-in models, it sets the reflection parameter used to evaluate the reflection probability (parameter k in Equation 11). For RFM models, it sets the name of the reflection function to use. Type: Number/Character Default: none Range: [0, 1] for built-in models
rotation	Sets either the rotation angle in the wafer coordinate system or whether the wafer rotates continuously. Type: Number/Character Default: 0 Range: [-180, 180] / [continuous] Unit: degree/none
s1	Sets the first sputter coefficient. Type: Number Default: none
s2	Sets the second sputter coefficient. Type: Number Default: none
selective_materials	Sets a list of materials on which the deposition can occur. If this list is empty, deposition occurs on all materials of the structure. Type: List Default: empty

Chapter 6: Input Commands

define_deposit_machine

Table 30 Parameters of *define_deposit_machine* command (Continued)

Parameter	Description
sputter_exponent	Sets the exponent used to characterize the angular distribution $\cos^m\theta$ of the sputtered material. The specified value must be an integer. Type: Number Default: none Range: $[1, \infty[$
sputter_rate	Sets the sputtering rate. The net deposition rate is equal to <code>rate - sputter_rate</code> . Type: Number Default: none Range: $[0, 2]$ Unit: $\mu\text{m min}^{-1}$
sputter_type	Sets the angular distribution type of the sputtered material. Options are: <ul style="list-style-type: none">• diffuse• reflective Type: Character Default: none
sticking	Sets the sticking probability of the deposition precursors. Type: Number Default: none Range: $[0, 1]$
surface_tension	Sets the surface tension of the film to be deposited with respect to the surrounding fluid. Type: Number Default: none Range: $[0, \infty[$ Unit: dyn/cm
temperature	Sets the absolute temperature of the electroplating process. Type: Number Default: none Range: $[0, \infty[$ Unit: K

Chapter 6: Input Commands

define_deposit_machine

Table 30 Parameters of define_deposit_machine command (Continued)

Parameter	Description
tilt	Sets the tilt angle. Type: Number Default: 0 Range: [0, 90] Unit: degree
viscosity	Sets the dynamic viscosity of the film to be deposited. Type: Number Default: none Range:]0, ∞[Unit: poise
yield	Sets the name of the yield function to use for the deposition machine. Type: Character Default: none
z	Sets the number of electrons involved in deposition reactions. Type: Number Default: 2 Range: [1, 2147483647]
z_alpha	Sets the number of electrons transferred in the rate-determining elementary reaction. Type: Number Default: 1 Range: [1, 2147483647]

Limitations

The following limitations or conditions apply:

- The rotation and tilt parameters do not support the radian measurement unit and are not supported when model=crystal, model=electrodeposition, or model=spin_on.
- There are only two possible numeric values of the parameter rotation when defining a machine to be used with a 2D structure. The numeric values are obtained by converting, if needed, the angles given by:

-slice_angle [deg] + 90°
-slice_angle [deg] - 90°

Chapter 6: Input Commands

define_deposit_machine

into the range [-180, 180] degrees. In these formulas, `slice_angle` denotes the slice angle of the structure, set by the `slice_angle` parameter of the `define_structure` command or stored in the loaded TDR file.

When the default value of the slice angle is used (-90), the possible values of `rotation` are 0 and 180 degrees, respectively, for a machine to be used with a 2D structure (see [Simulation Coordinate System on page 35](#) and [define_structure on page 360](#)).

- You can use `rotation=continuous` when defining a machine to be used with a 2D structure that uses a rate formula module (RFM) model supporting continuous rotation, independently of the value of the slice angle (see [Continuously Rotating and Tilted Structure Modeling on page 57](#), [Data Available for Rate Calculation on page 574](#), and [Chapter 11 on page 592](#)).

Examples

Define a machine named `simpledepo` for a silicon deposition process that uses the model `simple`, and set the anisotropy coefficient to 0.5, the curvature coefficient to 0.05 μm, and the deposition rate to 1 μm/minute:

```
define_deposit_machine anisotropy=0.5 curvature=0.05 \
    material=Silicon model=simple name=simpledepo rate=1
```

You can define the wafer plane tilt by using the tilt and rotation angles as described in [Structure Tilt on page 37](#).

The same example with a tilted structure is:

```
define_deposit_machine anisotropy=0.5 curvature=0.05 \
    material=Silicon model=simple name=simpledepo \
    rate=1 rotation=20 tilt=45
```

Chapter 6: Input Commands

define_diffuse_machine

define_diffuse_machine

This command defines a new machine for a diffusion process involving voids.

Syntax

```
define_diffuse_machine model=<c> \
    [curvature_prefactor=<c>] [field_names=<l>] [fields=<l>] \
    [formation_volume=<n>] [pressure=<c>] \
    [pressure_prefactor=<c>] [surface_diffusion_energy=<n>]
    [void_velocity_x=<c>] [void_velocity_y=<c>] [void_velocity_z=<c>]
```

Table 31 Parameters of *define_diffuse_machine* command

Parameter	Description
curvature_prefactor	Sets the curvature prefactor, which is $v_0 C$ from Equation 43 . This is an expression of x, y, z, t, and field_names (fields). Type: Character Default: none Range: $[0, \infty)$ Unit: $\text{m}^4 \text{K}$
field_names	Specifies a list of the variable names corresponding to the fields read from TDR files to be used in expressions for the parameters curvature_prefactor, pressure, pressure_prefactor, and void_velocity_*. If specified, then the number of field_names must correspond to the number of fields. Type: List Default: none
fields	Specifies a list of fields to be read from TDR files so they can be referred to expressions for the parameters curvature_prefactor, pressure, pressure_prefactor, and void_velocity_*. Aliases for TDR field names can be specified by using the field_names parameter. Type: List Default: none
formation_volume	Sets the formation volume. This is v_0 from Equation 42 . Type: Number Default: none Range: $[0, \infty)$ Unit: m^3

Chapter 6: Input Commands

define_diffuse_machine

Table 31 Parameters of define_diffuse_machine command (Continued)

Parameter	Description
model	Specifies the surface diffusion model. The only allowed value is mullins. Type: Character Default: mullins
pressure	Sets the pressure. This is P from Equation 43 . This is an expression of x , y , z , t , temperature, and field_names (fields). Type: Character Default: 0 Range: $[0, \infty)$ Unit: Pa
pressure_prefactor	Sets the pressure prefactor. This is $v_0 P$ from Equation 43 . This is an expression of x , y , z , t , and field_names (fields). Type: Character Default: none Range: $[0, \infty)$ Unit: m ² /s
surface_diffusion_energy	Sets the surface diffusion energy. This is E_d from Equation 43 . Type: Number Default: 0 Range: $[0, \infty)$ Unit: eV
void_velocity_x, void_velocity_y, void_velocity_z	As an alternative to pressure-dependent convection velocity (that is, the second term of Equation 43), these parameters can be used to specify expressions for the convection velocity directly. They can contain x , y , z , t , and field_names (fields). Type: Character Default: none Range: $(-\infty, \infty)$ Unit: m/s

Chapter 6: Input Commands

```
define_diffuse_machine
```

Examples

The following example creates a set of diffusion parameters (referred to as a machine) to be used with the `diffuse` command, which simulates surface diffusion and surface convection (see [diffuse on page 392](#)). The convection is either modeled as a flux of vacancies driven by a pressure gradient or specified directly by using `void_velocity_x`, `void_velocity_y`, and `void_velocity_z`. If specifying `pressure`, then it can be either specified as an expression of `x`, `y`, `z`, and `t` or read from external files using the `fields` parameter and related parameters of the `diffuse` command: `field_files` and `field_times`.

```
# Create a diffusion machine with constant diffusivity
# and no void velocity convection.
define_diffuse_machine \
    name=d1 \
    model=mullins \
    material=Silicon \
    curvature_prefactor=3e-2 \
    surface_diffusion_energy=1.0

diffuse \
    spacing=0.015 \
    machine=d1 \
    time=3<s> \
    temperature=1.0 \
    cfl=1000.0

# When specifying pressure in the diffuse command, you must set
# the formation volume of the vacancies in m^3; here 1.e-6
# converts cm^3 to m^3.
define_diffuse_machine \
    name=d2 \
    model=mullins \
    material=Silicon \
    curvature_prefactor=1.0e-5 \
    pressure_prefactor=1.0 \
    formation_volume=[expr 1.e-6 * 1.0/5.e22] \
    surface_diffusion_energy=4.0

diffuse spacing=50<nm> \
    machine=d2 \
    time=1<s> \
    temperature=1000.0 \
    pressure="1.e11*z"

# In this example, "Pressure" is read from fields_0.tdr and
# fields_1.tdr and is interpolated in space and time. The
# corresponding internal variable is named "pressure". The
# values of pressure, prefactors, and velocities are written
# to the diffuse_fields_inter.tdr file at the specified
# time (in seconds) during the diffuse step.
```

Chapter 6: Input Commands

define_diffuse_machine

```
define_diffuse_machine \
    name=d3 \
    model=mullins \
    material=Silicon \
    curvature_prefactor=3e-2 \
    formation_volume=2.000000000000002e-29 \
    surface_diffusion_energy=0.0 \
    fields="Pressure" \
    field_names="pressure" \
    pressure_prefactor=25

diffuse \
    spacing=0.015 \
    machine=d3 \
    cfl=1000 \
    time=0.15<s> \
    file=diffuse_fields_inter.tdr \
    plot_times="1e-5 1e-4 1e-3 1e-2 0.1 0.15" \
    plot_times_unit=s \
    temperature="1000.0" \
    field_times="0. 1.0" \
    field_files= { fields_0.tdr fields_1.tdr } \
    decimate=true \
    accuracy=0.02<um>
```

Chapter 6: Input Commands

define_electric_contact

define_electric_contact

This command defines an electric contact.

When simulating charge-up with a PMC model, you can use this command to assign a fixed potential to a conducting region in a structure.

Note:

If there is no conducting material at the specified position in the structure, then the command is ignored.

Syntax

```
define_electric_contact name=<c> position=<v> potential=<n>
```

Table 32 Parameters of *define_electric_contact* command

Parameter	Description
name	Sets the name of the electric contact to be referenced in the command <code>define_electric_solver</code> (see define_electric_solver on page 239). Type: Character Default: none
position	Sets the position of the point-like electric contact. The contact only takes effect if the position lies inside the conducting material. Conducting material can be defined in the command <code>define_species_properties</code> . Type: Vector Default: none Range: $(-\infty, \infty) \times (-\infty, \infty) \times (-\infty, \infty)$ Unit: μm
potential	Sets the potential applied to the conducting material at the electric contact. Type: Number Default: none Range: $(-\infty, \infty)$ Unit: V

Chapter 6: Input Commands

define_electric_solver

define_electric_solver

This command defines an electric solver.

When simulating charge-up with a PMC model, you can use this command to configure the Poisson solver for computing the electric field.

Note:

This command is optional. If you do not define the electric solver explicitly, then the default values are used for the charge-up simulation.

Syntax

```
define_electric_solver name=<c> \
    [grc_grid_refinement_ratio=<n>] \
    [grc_max_num_iterations=<n>] \
    [grc_preconditioner=<c>] \
    [grc_solver=<c>] \
    [grc_solver_abs_error=<n>] \
    [grc_solver_optimization=<b>] \
    [grc_solver_rel_error=<n>]
```

Table 33 Parameters of *define_electric_solver* command

Parameter	Description
grc_grid_refinement_ratio	Sets the mesh size of the Poisson solver grid in units of the PMC grid spacing. Type: Number Default: 1 Range: $[1, \infty)$
grc_max_num_iterations	Sets the maximum number of iterations for the Poisson solver to converge to the solution. Type: Number Default: 10000000 Range: $[1, \infty)$
grc_preconditioner	Selects the preconditioner used by the Poisson solver to prepare the linear matrix. Options are: <ul style="list-style-type: none">• spai0_preconditioner• ilu0_preconditioner• ilut_preconditioner• no_preconditioner Type: Character Default: spai0_preconditioner

Chapter 6: Input Commands

define_electric_solver

Table 33 Parameters of define_electric_solver command (Continued)

Parameter	Description
grc_solver	<p>Selects the linear solver used by Poisson solver to compute the electric potential. Options are:</p> <ul style="list-style-type: none"> • bicgstab_solver • cg_solver • cgs_solver • cgs2_solver • gmres_solver <p>Type: Character Default: bicgstab_solver</p>
grc_solver_abs_error	<p>Sets the convergence threshold for the iterative linear solver for the electric potential, used by the Poisson solver. The absolute error is defined as the residuum of the linear equation system.</p> <p>Type: Number Default: 0 Range: $[0, \infty)$</p>
grc_solver_optimization	<p>Specifies whether to dynamically select the linear solver and preconditioner to optimize robustness and performance. (If switched on, then the values of grc_solver and grc_preconditioner are used as initial solvers or preconditioners, but they can change during the simulation.)</p> <p>Type: Boolean Default: true</p>
grc_solver_rel_error	<p>Sets the convergence threshold for the iterative linear solver for the electric potential, used by the Poisson solver. The relative error is defined as the relative residuum of the linear equation system (that is, the final residuum divided by the initial residuum).</p> <p>Type: Number Default: $1e-8$ Range: $[0, \infty)$</p>
name	<p>Sets the name of the electric solver object. This name is referenced in the etch command.</p> <p>Type: Character Default: none</p>

Chapter 6: Input Commands

define_electric_solver

Examples

```
define_electric_solver name=cp \
    grc_grid_refinement_ratio=4 \
    grc_solver=cgs_solver \
    grc_preconditioner=ilu0_preconditioner \
    grc_solver_abs_error=1e-6 \
    grc_max_num_iterations=100000000
```

Chapter 6: Input Commands

define_etch_machine

define_etch_machine

This command defines a new machine for an etching model, or a simultaneous etching and deposition model, or a deposition reaction model. Parameters defined with the define_etch_machine command are material independent except when setting model=crystal.

Material-dependent parameters are defined with the add_material command. When setting model=crystal, the specified etching rates refer to the single etchable material. The add_material command cannot be used with a machine having model=crystal.

Syntax

Crystal orientation-dependent etching:

```
define_etch_machine etchable_material=<c> model=crystal \
    rate_100=<n> rate_110=<n> rate_111=<n> \
    [name=<c>] [pattern_density_model=<c>]
```

Dry etching:

```
define_etch_machine deposit_material=<c> model=dry \
    rate=<n> sticking=<n> \
    [nad=<c> | neutral_exponent=<n>] [name=<c>] \
    [pattern_density_model=<c>] [rotation=<n>] [tilt=<n>]
```

Simultaneous etching and deposition:

```
define_etch_machine (exponent=<n> | iad=<c>) deposit_material=<c> \
model=etchdepo rate=<n> sticking=<n> \
    [name=<c>] [pattern_density_model=<c>] [rotation=<n>] [tilt=<n>]
```

Simultaneous etching and deposition 2:

```
define_etch_machine (exponent=<n> | iad=<c>) deposit_material=<c> \
model=etchdepo2 rate=<n> sticking=<n> \
    [nad=<c> | (neutral_etch_exponent=<n> | neutral_exponent=<n>)] \
    [name=<c>] [pattern_density_model=<c>] [rotation=<n>] [tilt=<n>]
```

High-density plasma etching:

```
define_etch_machine (exponent=<n> | iad=<c>) model=hdp \
    [name=<c>] [pattern_density_model=<c>] [rotation=<n>] [tilt=<n>]
```

High-density plasma 2 etching:

```
define_etch_machine (exponent=<n> | iad=<c>) model=hdp2 \
    [nad=<c> | neutral_exponent=<n>] [name=<c>] \
    [pattern_density_model=<c>] [rotation=<n>] [tilt=<n>]
```

Chapter 6: Input Commands

```
define_etch_machine
```

Ion-enhanced etching:

```
define_etch_machine (exponent=<n> | iad=<c>) model=ion_enhanced \
[nad=<c> | neutral_exponent=<n>] [name=<c>] \
[pattern_density_model=<c>] [rotation=<n>] [tilt=<n>]
```

Ion-milling:

```
define_etch_machine model=ionmill [name=<c>] \
[pattern_density_model=<c>] [rotation=<n>] [tilt=<n>]
```

Reactive ion etching:

```
define_etch_machine (exponent=<n> | iad=<c>) model=rie \
[name=<c>] [pattern_density_model=<c>] [rotation=<n>] [tilt=<n>]
```

Reactive ion etching 2:

```
define_etch_machine (exponent=<n> | iad=<c>) model=rie2 \
[nad=<c> | neutral_exponent=<n>] [name=<c>] \
[pattern_density_model=<c>] [rotation=<n>] [tilt=<n>]
```

Simple etching:

```
define_etch_machine model=simple [name=<c>] \
[pattern_density_model=<c>] [rotation=<n>] [tilt=<n>]
```

Wet etching:

```
define_etch_machine diffusivity=<n> model=wet source_distance=<n> \
[name=<c>] [pattern_density_model=<c>] [source_concentration=<n>]
```

RFM model:

```
define_etch_machine model=<c> [applied_pressure=<n>] \
[deposit_material=<c>] [iad=<c>] [maximum_error=<n>] [nad=<c>] \
[name=<c>] [pad_poisson_ratio=<n>] [pad_roughness=<n>] \
[pad_young_modulus=<n>] [pattern_density_model=<c>] \
[reflection=<c>] [rotation=<n> | <c>] [tilt=<n>] [yield=<c>] ...
```

Reaction model:

```
define_etch_machine model=<c> species_distribution=<c> \
[charging_model=<c>] [damage=<c>] [name=<c>] \
[pattern_density_model=<c>] \
[rotation=<n> | <c>] [species_properties=<c>] \
[source_position=<n>] [surface_transport_model=<c>] [tilt=<n>] \
[top_plane_distance=<n>] [volumetric_species_distribution=<c>] \
[yield=<c>]
```

Chapter 6: Input Commands

define_etch_machine

Table 34 Parameters of define_etch_machine command

Parameter	Description
applied_pressure	Sets the external pressure applied to the pad. It is mandatory for RFM models using the RFM function <code>pad_pressure()</code> . Type: Number Default: none Range: $[0, \infty[$ Unit: Pa
charging_model	When simulating charge-up, this parameter sets the name of the charging model, defined by the <code>define_charging_model</code> command (see define_charging_model on page 213). Type: Character Default: none
damage	You can use this optional parameter with the reaction model that is available for PMC steps. It switches on the accumulation of damage by naming profiles created with the <code>define_damage</code> command (see define_damage on page 217). Type: Character Default: none
deposit_material	Sets the deposition material for simultaneous etching and deposition models. Type: Character Default: none
diffusivity	Sets the diffusivity of the etchant species. Type: Number Default: none Range: $]0, \infty[$ Unit: cm^2/s
etchable_material	Sets the material to be etched. Type: Character Default: none
exponent	Sets the exponent used to characterize the ion angular distribution $\cos^m\theta$. Type: Number Default: none Range: $[1, \infty[$

Chapter 6: Input Commands

define_etch_machine

Table 34 Parameters of define_etch_machine command (Continued)

Parameter	Description
iad	Sets the name of the IAD to be used. Type: Character Default: none
maximum_error	Sets the maximum tolerated equivalence error for all species of the model. This parameter can be used only if <code>rotation=continuous</code> . See Continuously Rotating and Tilted Structure Modeling on page 57 . Type: Number Default: 0.5 Range: [0, 0.5]
model	Sets the model used to represent the physical machine. Type: Character Default: none
nad	Sets the name of the NAD to be used. Type: Character Default: none
name	Sets the name of the etch machine. Type: Character Default: default_machine
neutral_etch_exponent	Sets the exponent used to characterize the angular distribution $\cos^m\theta$ of the etching neutral flux ($\Gamma_{\text{neutral etch}}$ in Equation 39 of the model <code>etchdepo2</code>). Note: This parameter is available only when <code>model=etchdepo2</code> . Type: Number Default: 1 Range: [1, ∞[
neutral_exponent	Sets the exponent used to characterize the neutral angular distribution $\cos^m\theta$. When <code>model=etchdepo2</code> , this parameter refers to the deposition neutral flux (Γ_{neutral} in Equation 39). Type: Number Default: 1 Range: [1, ∞[

Chapter 6: Input Commands

define_etch_machine

Table 34 Parameters of define_etch_machine command (Continued)

Parameter	Description
pad_poisson_ratio	Sets the Poisson ratio of the pad. It is mandatory for RFM models using the RFM function <code>pad_pressure()</code> . Type: Number Default: none Range:]-1, 0.5]
pad_roughness	This parameter is related to the standard deviation of the distribution of the pad asperities. It is mandatory for RFM models using the RFM function <code>pad_pressure()</code> . Type: Number Default: none Range:]0, ∞ [Unit: μm
pad_young_modulus	Sets the Young's modulus of the pad. It is mandatory for RFM models using the RFM function <code>pad_pressure()</code> . Type: Number Default: none Range:]0, ∞ [Unit: Pa
pattern_density_model	Sets the pattern density model defined in the command <code>define_pattern_density_model</code> (see define_pattern_density_model on page 295). This parameter can be used only for level set models. Type: Character Default: none
rate	Sets the rate of deposition for the material that was specified with the <code>deposit_material</code> parameter. Type: Number Default: none Range:]0, ∞ [Unit: $\mu\text{m min}^{-1}$
rate_100	Sets the etching rate for the <100> direction. Type: Number Default: none Range:]0, ∞ [Unit: $\mu\text{m min}^{-1}$

Chapter 6: Input Commands

define_etch_machine

Table 34 Parameters of define_etch_machine command (Continued)

Parameter	Description
rate_110	Sets the etching rate for the <110> direction. Type: Number Default: none Range: [0, ∞[Unit: $\mu\text{m min}^{-1}$
rate_111	Sets the etching rate for the <111> direction. Type: Number Default: none Range: [0, ∞[Unit: $\mu\text{m min}^{-1}$
reflection	Sets the name of the reflection function to be used. Type: Character Default: none
rotation	Sets either the rotation angle in the wafer coordinate system or whether the wafer rotates continuously. Type: Number / Character Default: 0 Range: [-180, 180] / continuous Unit: degree / none
source_concentration	Sets the concentration of the etchant species on the source plane. Type: Number Default: 1 Range:]0, ∞[Unit: mol/cm ³
source_distance	Sets the distance of the plane where the etchant concentration is assumed to be fixed from the topmost point of the exposed surface. Type: Number Default: none Range:]0, ∞[Unit: μm

Chapter 6: Input Commands

define_etch_machine

Table 34 Parameters of *define_etch_machine* command (Continued)

Parameter	Description
source_position	If specified, the z-coordinate of the particle source in the PMC simulator is fixed to this height. Otherwise, the position of the source is adjusted dynamically to keep a fixed distance to the structure top during the simulation. Note: The source position must lie inside the simulation bounding box. To extend the bounding box in the vertical direction, use the command <code>fill material=Gas thickness=<n></code> , or use the <code>top_gas_thickness</code> parameter in the <code>etch</code> or <code>filter_structure</code> command. Type: Number Default: none Unit: μm
species_distribution	Sets the name of the species distribution to be used. Note: This parameter must be specified if the model set by the parameter <code>model</code> is a reaction model containing source species defined using the <code>add_source_species</code> command (see add_source_species on page 203). Type: Character Default: none
species_properties	Sets the name of the species properties to be used. Type: Character Default: none
sticking	Sets the sticking coefficient for the deposition material that was specified with the parameter <code>deposit_material</code> . Type: Number Default: none Range: [0, 1]
surface_transport_model	Sets the name of the surface transport model to be used. Type: Character Default: none

Chapter 6: Input Commands

define_etch_machine

Table 34 Parameters of *define_etch_machine* command (Continued)

Parameter	Description
tilt	Sets the tilt angle. Type: Number Default: 0 Range: [0, 90] Unit: degree
top_plane_distance	Sets the distance between the (dynamic) top plane and the exposed surface of the structure. This parameter can be used only for top plane reactions (see Example of Top Plane Reactions on page 187). Type: Number Default: none Range:]0, ∞] Unit: μm
volumetric_species_distribution	Sets the name of the volumetric species distribution to be used. Note: This parameter must be specified if the model set by the parameter <code>model</code> is a reaction model containing volumetric source species defined using the <code>add_volumetric_source_species</code> command (see add_volumetric_source_species on page 206). Type: Character Default: none
yield	Sets the name of the yield function to be used. Type: Character Default: none

Limitations

The following limitations or conditions apply:

- The `rotation` and `tilt` parameters do not support the radian measurement unit and are not supported when `model=crystal` or `model=wet`.

Chapter 6: Input Commands

define_etch_machine

- There are only two possible numeric values of the parameter `rotation` when defining a machine to be used with a 2D structure. The numeric values are obtained by converting, if needed, the angles given by:

-slice_angle [deg] + 90°
-slice_angle [deg] - 90°

into the range [-180, 180] degrees. In these formulas, `slice_angle` denotes the slice angle of the structure, set by the `slice_angle` parameter of the `define_structure` command or stored in the loaded TDR file.

When the default value of the slice angle is used (-90), the possible values of `rotation` are 0 and 180 degrees for a machine to be used with a 2D structure (see [Simulation Coordinate System on page 35](#) and [define_structure on page 360](#)).

- You can use `rotation=continuous` when defining a machine to be used with a 2D structure that uses a rate formula module (RFM) model supporting continuous rotation, independently of the value of the slice angle (see [Continuously Rotating and Tilted Structure Modeling on page 57](#), [Data Available for Rate Calculation on page 574](#), and [Chapter 11 on page 592](#)).
- When defining a machine that uses a reaction model, you can use `rotation=continuous` only if no source species of the reaction model has an energy-dependent distribution computed by HPEM, the Benoit-Cattin plasma sheath model, or the Edelberg–Aydil plasma sheath model, or imported from an EAD file (see [define_species_distribution on page 337](#)).
- When defining an etch machine that uses a reaction model, only two cases are supported:
 - The species distributions specified for all the source species of the used reaction models are energy independent. In this case, also the yield functions required by the reaction model and its reaction probabilities must be energy independent.
 - The species distributions specified for all the source species of the used reaction models are energy dependent. In this case, the yield functions required by the reaction model and its reaction probabilities can be either energy independent or energy dependent.

In all other cases, an error will be issued.

Examples

Define a machine named `etchmachine` for an etching process that uses the model `simple`:

```
define_etch_machine name=etchmachine model=simple
```

You can define the wafer plane tilt by using the `tilt` and `rotation` angles as described in [Structure Tilt on page 37](#).

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define_etch_machine

The same example with a tilted structure is:

```
define_etch_machine name=etchmachine model=simple rotation=45 tilt=30
```

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define_extraction

define_extraction

This command allows you to define extractions that can be used during a deposition step or an etching step or a plasma simulation.

Extractions for Deposition and Etching Simulations

This section describes the `define_extraction` command for deposition and etching simulations.

Syntax

Define the extraction of an interface between two different materials, or two different regions, or two different parts along a line in a structure:

```
define_extraction name=<c> type=interface <extraction_line> \
    <extraction_pair> tcl_output_variable=<c> \
    [description=<c>] [output=<c>]
```

Define the extraction of a property of a structure along a line:

```
define_extraction name=<c> type=probe property=length \
    <extraction_line> (materials=<l> | [probe_empty_space=<b>]) \
    [description=<c>] [file=<c>] [output=<c>] [tcl_output_variable=<c>]

define_extraction name=<c> type=probe property=<c> \
    <extraction_line> tcl_output_variable=<c> \
    [description=<c>] [output=<c>]
```

With the following command, you can define the extraction of several PMC quantities in a given bounding box:

- Number of executed reactions
- Volume of the specified species
- Volume deposited or sputtered according to the specified reactions
- Effective sputter yield of the specified reactions
- Volume density of the starting points of the volumetric source species
- When simulating charge-up, the charge density, the electric field, and the electric potential

```
define_extraction type=pmc_data name=<c> quantities=<l> \
    [axis=<c> position=<n> [crop_plane=<b>]] [csv_file=<c>] \
    [description=<c>] \
    [expression_pattern=<c> | reactions=<l>] \
    [file=<c>] [grid_output=<b>] [normalization=<c>] \
```

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define_extraction

```
[operator=<c>] [point_max=<v> point_min=<v>] \
[species=<l>] [tdr_dataset_grouping=<c>] \
[tcl_output_variable=<c>]
```

Note:

The `pmc_data` extraction type is available only for PMC simulations.

Define the extraction of ion and neutral trajectory paths during a charge-up simulation:

```
define_extraction name=<c> type=trajectories \
[csv_file=<c>] [description=<c>] \
[end_point_min=<v> end_point_max=<v>] \
[energy_min=<n> energy_max=<n>] \
[file=<c>] \
[num_trajectories=<n> | start_point_spacing=<n>] \
[species=<l>] \
[start_point_min=<v> start_point_max=<v>] \
[tcl_output_variable=<c>]
```

In this syntax:

- You can specify a list of ion and neutral species names to be extracted (parameter `species`).
- You can specify the number of trajectories (parameter `num_trajectories`) or, alternatively, the spacing between their start positions (parameter `start_point_spacing`).
- You can restrict the start positions to a sub-area (parameters `start_point_min` and `start_point_max`).
- You can extract only trajectories ending in a certain subvolume (parameters `end_point_min` and `end_point_max`).
- You can extract only trajectories within a certain energy window (parameters `energy_min` and `energy_max`).

Define the extraction of the intersection of a 3D boundary or PMC structure with a plane:

```
define_extraction type=slice <extraction_plane> name=<c> \
[description=<c>] [file=<c>] [tcl_output_variable=<c>]
```

In this syntax:

- An extraction line specification `<extraction_line>`, as defined in the `extract` command, specifies the location at which the extraction is performed.
- An extraction pair specification `<extraction_pair>`, as defined in the `extract` command, specifies a pair of materials, or parts, or regions for which the extraction is performed.

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define_extraction

- An extraction plane specification <extraction_plane>, as defined in the extract command, specifies the plane in which the extraction is performed.

Table 35 Parameters of *define_extraction* command

Parameter	Description
axis ^{1 2}	Sets the direction of one of the coordinate axes. Options are: <ul style="list-style-type: none">xyz Type: Character Default: none
crop_plane	Specifies whether or not to limit the 2D results to the portion of the specified plane that intersects the bounding box specified by point_max and point_min. If the specified plane does not intersect the given bounding box, then an error is issued. Type: Boolean Default: false
csv_file	Sets the name of the CSV file where to write the extracted scalar results in CSV format. If omitted, no CSV output is produced. If the specified file already exists when the first extraction is performed, then it is overwritten. Note: If multiple define_extraction commands with the same name value use the same value for the csv_file parameter, then an error is issued. Type: Character Default: none
description	Describes the extraction. Type: Character Default: none
direction ¹	Sets the direction of the extraction line. Type: Vector Default: none

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define_extraction

Table 35 Parameters of define_extraction command (Continued)

Parameter	Description
end_point_max	<p>Sets the upper-right corner point of the cuboid in which the trajectories end. Only trajectories ending in the specified volume are extracted. This parameter is available only when type=trajectories.</p> <p>Note: Trajectories can end only at the surface or in the plasma.</p> <p>Type: 3D vector Default: The upper-right corner point of the bounding box of the structure to which the defined extraction is applied Unit: μm</p>
end_point_min	<p>Sets the lower-left corner point of the cuboid in which the trajectories end. Only trajectories ending in the specified volume are extracted. This parameter is available only when type=trajectories.</p> <p>Note: Trajectories can end only at the surface or in the plasma.</p> <p>Type: 3D vector Default: The lower-left corner point of the bounding box of the structure to which the defined extraction is applied Unit: μm</p>
energy_max	<p>Sets the upper boundary of the energy window from which trajectories will be sampled. This parameter is available only when type=trajectories.</p> <p>Type: Number Default: none Range:]0, ∞[Unit: eV</p>
energy_min	<p>Sets the lower boundary of the energy window from which trajectories will be sampled. This parameter is available only when type=trajectories.</p> <p>Type: Number Default: none Range:]0, -∞[Unit: eV</p>

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define_extraction

Table 35 Parameters of define_extraction command (Continued)

Parameter	Description
expression_pattern	<p>Sets the search pattern of the reaction expression that specifies for which reactions the results must be extracted. The search pattern must be given in the glob syntax.</p> <p>Results are extracted for all reactions with an expression that matches the specified search pattern.</p> <p>In any case, the set of matching reactions:</p> <ul style="list-style-type: none">• Must not be empty• Must contain either only top plane reactions or no top plane reactions <p>You can specify this parameter when the parameter <code>quantities</code> contains the value <code>deposited_volume</code>, <code>reaction_executions</code>, <code>sputtered_volume</code>, or <code>sputter_yield</code>.</p> <p>When it denotes top plane reactions, the parameter <code>quantities</code> must contain only the value <code>reaction_executions</code>.</p> <p>Type: Character Default: none</p>
file	<p>Sets the file name or path to a file where the extraction results will be saved.</p> <p>Type: Character Default: none</p>
grid_output	<p>Specifies whether or not to produce 3D results.</p> <p>Type: Boolean Default: false</p>
material ³	<p>Sets the name of the first material of an extraction pair specification.</p> <p>Type: Character Default: none</p>
material2 ³	<p>Sets the name of the second material of an extraction pair specification.</p> <p>Type: Character Default: none</p>
materials	<p>Sets the materials to take into account.</p> <p>Note: This parameter applies only if <code>property=length</code>.</p> <p>Type: List Default: none</p>

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define_extraction

Table 35 Parameters of define_extraction command (Continued)

Parameter	Description
name	Sets the name of the extraction group to which the extraction is added. Type: Character Default: none
normal ²	Sets the normal of the specified plane. Type: Vector Default: none
normalization	Sets how to normalize the sum of the extracted quantities over the boundary box. Options are: <ul style="list-style-type: none">• none• box When normalization=box, the sum of the quantity values collected in the given bounding box, divided by the bounding box volume (area), is computed. When normalization=none, the sum of the quantity values collected in the given bounding box is computed. Type: Character Default: none
num_trajectories	Sets the number of trajectories to be extracted. The start positions of the trajectories are random. If you want regularly spaced start positions, then use the parameter start_point_spacing instead. This parameter is available only when type=trajectories. You can specify either num_trajectories or start_point_spacing. Type: Number Default: 50

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define_extraction

Table 35 Parameters of define_extraction command (Continued)

Parameter	Description
operator	<p>Sets the mathematical operation to reduce the 3D volume data to a scalar value for the quantities specified by the parameter <code>quantities</code>. Reduction operators are available for the quantities <code>charge_density</code>, <code>electric_field</code>, and <code>electric_potential</code>:</p> <ul style="list-style-type: none">• <code>integral</code>• <code>mean</code>• <code>max</code>• <code>meanabs</code>• <code>min</code>• <code>stddev</code>• <code>sum</code>• <code>sumabs</code> <p>Type: Character Default: mean</p>
output	<p>Sets a filtering option. Options are:</p> <ul style="list-style-type: none">• <code>all</code>• <code>first</code>• <code>inside</code>• <code>last</code>• <code>outside</code> <p>Type: Character Default: all</p>
point_max	<p>Sets the requested maximum corner of the bounding box where the data must be extracted. It can be set only when <code>type=pmc_data</code>. The actual maximum corner of the bounding box where the data must be extracted is obtained by snapping the given <code>point_max</code> value to the closest grid point of the PMC structure on which the extraction is executed.</p> <p>Type: Vector Default: If <code>reactions</code> or <code>expression_pattern</code> denotes top plane reactions: <code>{∞ ∞}</code> Otherwise or when neither <code>reactions</code> nor <code>expression_pattern</code> is specified: <code>{∞ ∞ ∞}</code> Unit: μm</p>

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define_extraction

Table 35 Parameters of define_extraction command (Continued)

Parameter	Description
point_min	<p>Sets the requested minimum corner of the bounding box where the data must be extracted. It can be set only when type=pmc_data.</p> <p>The actual minimum corner of the bounding box, where the data must be extracted, is obtained by snapping the given point_min value to the closest grid point of the PMC structure on which the extraction is executed.</p> <p>Type: Vector</p> <p>Default: If reactions or expression_pattern denotes top plane reactions: { -∞ -∞ }</p> <p>Otherwise or when neither reactions nor expression_pattern is specified: { -∞ -∞ -∞ }</p> <p>Unit: μm</p>
point ^{1 2}	<p>Sets a point on the extraction line or plane.</p> <p>Type: Vector</p> <p>Default: none</p> <p>Unit: μm</p>
point1 ^{1 2}	<p>Sets the first point on the extraction line or plane.</p> <p>Type: Vector</p> <p>Default: none</p> <p>Unit: μm</p>
point2 ^{1 2}	<p>Sets the second point on the extraction line or plane.</p> <p>Type: Vector</p> <p>Default: none</p> <p>Unit: μm</p>
point3 ²	<p>Sets the third point on the extraction plane.</p> <p>Type: Vector</p> <p>Default: none</p> <p>Unit: μm</p>
position ²	<p>Sets the cutting plane distance from the origin measured in the direction defined by axis.</p> <p>Type: Number</p> <p>Default: none</p> <p>Unit: μm</p>

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define_extraction

Table 35 Parameters of define_extraction command (Continued)

Parameter	Description
probe_empty_space	<p>Specifies whether or not to probe empty space.</p> <p>Note: This parameter applies only if <code>property=length</code>.</p> <p>Type: Boolean Default: false</p>
property	<p>Sets the property to be associated with the returned segments. Options are:</p> <ul style="list-style-type: none">• length• material• region• region_part <p>Note: You can use <code>property=region</code> and <code>property=region_part</code> only during a deposition step or an etching step using <code>method=levelset</code>.</p> <p>Type: Character Default: none</p>
quantities	<p>Specifies the quantities to extract. Options are:</p> <ul style="list-style-type: none">• charge_density• deposited_volume• electric_field• electric_potential• reaction_executions• species_volume• sputter_yield• sputtered_volume• volumetric_source_particles <p>Note: When you specify <code>volumetric_source_particles</code>, there must be a volumetric source species in the used model.</p> <p>Type: List Default: none</p>

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define_extraction

Table 35 Parameters of define_extraction command (Continued)

Parameter	Description
reactions	<p>Sets the names of the reactions for which results must be extracted. The following conditions apply:</p> <ul style="list-style-type: none"> • The list must not be empty. • The list must contain either only top plane reactions or no top plane reactions. • All listed reactions must exist in the model of the etch machine used by the <code>etch</code> command that uses this extraction. <p>You can specify this parameter when <code>quantities</code> contains the value <code>deposited_volume</code>, <code>reaction_executions</code>, <code>sputtered_volume</code>, or <code>sputter_yield</code>.</p> <p>When it denotes top plane reactions, the parameter <code>quantities</code> must contain only <code>reaction_executions</code>.</p> <p>Type: List Default: none</p>
region_part1 ³	<p>Sets the names of the first region and part in an extraction pair specification.</p> <p>Type: List Default: none</p>
region_part2 ³	<p>Sets the names of the second region and part in an extraction pair specification.</p> <p>Type: List Default: none</p>
region1 ³	<p>Sets the name of the first region in an extraction pair specification.</p> <p>Type: Character Default: none</p>
region2 ³	<p>Sets the name of the second region in an extraction pair specification.</p> <p>Type: Character Default: none</p>
species	<p>Sets the names of the species to be extracted. This parameter can be specified only when extracting <code>charge_density</code> or <code>trajectories</code>. When extracting <code>trajectories</code>, the ratio between the number of trajectories for each species corresponds to the flux ratio.</p> <p>Type: List Default: All species extracted; when <code>type=trajectories</code>, all species are sampled according to their flux ratio</p>

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`define_extraction`

Table 35 Parameters of `define_extraction` command (Continued)

Parameter	Description
<code>start_point_max</code>	<p>Sets the area on the top plane from which the trajectories are started. This parameter is available only when <code>type=trajectories</code>.</p> <p>Type: 2D vector</p> <p>Default: The x- and y-coordinates of the upper-right corner point of the bounding box of the structure to which the defined extraction is applied</p> <p>Unit: μm</p>
<code>start_point_min</code>	<p>Sets the area on the top plane from which the trajectories are started. This parameter is available only when <code>type=trajectories</code>.</p> <p>Type: 2D vector</p> <p>Default: The x- and y-coordinates of the lower-left corner point of the bounding box of the structure to which the defined extraction is applied</p> <p>Unit: μm</p>
<code>start_point_spacing</code>	<p>Sets the regular spacing between the start positions of the trajectories in the xy plane. This parameter is available only when <code>type=trajectories</code>. You can specify either <code>num_trajectories</code> or <code>start_point_spacing</code>.</p> <p>Type: Number</p> <p>Default: none</p> <p>Unit: μm</p>
<code>tcl_output_variable</code>	<p>Sets the name of the Tcl variable to which the extraction results will be written.</p> <p>If omitted, no Tcl output is produced.</p> <p>If the specified Tcl variable already exists when the first extraction is performed, then its value is overwritten.</p> <p>Note: If multiple <code>define_extraction</code> commands with the same <code>name</code> value use the same value for <code>tcl_output_variable</code>, then an error message is issued.</p> <p>Type: Character</p> <p>Default: none</p>

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define_extraction

Table 35 Parameters of define_extraction command (Continued)

Parameter	Description
tdr_file_dataset_grouping	<p>Specifies how to group the datasets in the TDR file for plotting in Sentaurus Visual. This parameter only affects the 1D function output of type pmc_data. Options are:</p> <ul style="list-style-type: none">pmc_data: Datasets are all labeled with a pmc_data tag.quantity: Datasets are labeled with the respective quantity name. <p>Type: Character Default: pmc_data</p>
type	<p>Sets the extraction type. Options are:</p> <ul style="list-style-type: none">interfacepmc_dataprobeslicetrajectories <p>Note: The pmc_data extraction type is available only for PMC simulations.</p> <p>Type: Character Default: none</p>

1. Parameter specifies an extraction line (see [Specifying Extraction Lines, Planes, and Pairs on page 438](#)).
2. Parameter specifies an extraction plane (see [Specifying Extraction Lines, Planes, and Pairs on page 438](#)).
3. Parameter specifies an extraction pair (see [Specifying Extraction Lines, Planes, and Pairs on page 438](#)).

Description

When using the define_extraction command:

- Each extraction defined with the define_extraction command is added to the group of extractions specified with the parameter name.
- To use a group of extractions defined with the define_extraction command in the deposit or etch command, the name of the extraction group is specified with the extraction parameter, and the time interval at which the extractions are performed is specified with the extraction_interval parameter. See [deposit on page 375](#) and [etch on page 399](#).
- Except for those with type=pmc_data, extractions defined with the define_extraction command work in a similar way to corresponding extractions defined with the extract command.

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define_extraction

- Each extraction defined with the `define_extraction` command can write its output to a Tcl variable, whose name is provided by the parameter `tcl_output_variable`.
- Except when `type=pmc_data`, the Tcl variable into which the extraction results are written is a list of values with the following format:

```
t_0 extraction_result_0 t_1 extraction_result_1 ...
```

where:

- `t_i` is the *i*-th extraction time in minutes.
- `extraction_result_i` is the result of an intermediate extraction.

When `quantities` is set to `deposited_volume`, `reaction_executions`, and `sputtered_volume`, it is a list of `{reaction_name extracted_value}` pairs.

In other cases, `extraction_result_i` is the result that the corresponding `extract` command would produce if run on the structure at time `t_i`.

- When `type=pmc_data`, the Tcl variable into which the extraction results are written is a list of values with the following format:

```
headers data
```

where:

- `headers` is a list of extracted value names, including the extraction time, which is the first element (`time`).
 - `data` is a list of extracted values, including the extraction time, given in the order specified by `headers`.
- When specifying `type=probe property=length`, the extraction output can also be written to a TDR file such that it can be visualized in Sentaurus Visual.

Note:

When using `model=pmc` in the `etch` command, if both the `extraction_interval` and `plot_interval` parameters are specified, their values must be the same.

Examples

```
define_extraction name=extr axis=z point={0.2 0.2 0} type=probe \
    property=length materials=Silicon file=output.tdr

define_extraction name=extr axis=z point={0.2 0.2 1} type=interface \
    tcl_output_variable=res

etch time=1 spacing=0.1 extraction_interval=0.1 extraction=extr

puts "res = $res"
```

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```
define_extraction
```

In the first command, an extraction of type `probe` is added to the extraction group named `extr`. This will extract the vertical thickness of the material `Silicon` at the specified point and write the value to the specified TDR file.

In the second command, an extraction of type `interface` is added to the extraction group named `extr`. This will extract the position of an interface, and the result is assigned to the variable `res`.

The extraction group named `extr` is used every 0.1 minutes.

In the fourth line, the Tcl command `puts` is used to output the result of the interface extraction.

```
define_extraction name=extr type=pmc_data \
    quantities=deposited_volume \
    expression_pattern={R1 R2} tcl_output_variable=depo_vol_res \
    csv_file=depo_vol.csv

define_extraction name=extr type=pmc_data \
    quantities=reaction_executions \
    expression_pattern="*= $B< s >$ *" \
    tcl_output_variable=B_reactant_res file=B_reactant.tdr

etch method=pmc spacing=0.05 time=1 extraction_interval=0.2 \
    extraction=extr
```

In the first command, an extraction of quantity `deposited_volume` is added to the extraction group named `extr`. This extracts the volume deposited according to reactions `R1` and `R2`. The result will be assigned to the `depo_vol_res` variable, and it will be written to the CSV file `depo_vol.csv` and to the TDR file `<base_name>.tdr`.

In the second command, an extraction of quantity `reaction_executions` is added to the extraction group named `extr`. This extracts the number of executions of the reactions that have an expression matching the pattern `*= $B< s >$ *`, that is, those having `B< s >` as a reaction product. There must exist at least one reaction with a `B< s >` product in the model used by the `etch` command; otherwise, an error is issued. The result will be assigned to the variable `B_reactant_res` as well as written to the TDR file `B_reactant.tdr`.

The extraction group named `extr` is used every 0.2 minutes.

Extractions for Plasma Simulations

This section describes the `define_extraction` command for plasma simulations.

For plasma simulations, this command allows you to extract and monitor several plasma quantities, such as bulk densities, electron temperature, plasma reaction statistics,

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define_extraction

convergence residuals, electron energy distribution, and sheath characteristics (potential waveform, sheath currents, sheath capacitance, flux, electric field, and so on).

Syntax

```
define_extraction name=<c> type=plasma \
    (bulk_model_type=<c> | sheath_model_type=<c>) \
    [csv_file=<c>] \
    [expression_pattern=<c> | reactions=<l>] \
    [extraction_step=<n> | time_step=<n>] \
    [file=<c>] [file_update_step=<n>] \
    [log_file_update=<b>] [max_num_samples=<n>] [mode=<c>] \
    [output_type=<l>] [pattern_type=<c>] \
    [quantities=<l>] [regex_syntax=<c>] \
    [species=<l> | species_pattern=<c>]
```

Table 36 Parameters of *define_extraction* command for type=plasma

Parameter	Description
bulk_model_type	Sets the type of the bulk model. Depending on the bulk model type, different extraction quantities are available (see Table 37). The only option is global. Type: Character Default: none
csv_file	Sets the name of the CSV file. You can specify this parameter only for CSV-exportable quantities (see Table 37) and if <code>output_type=csv</code> . Type: Character Default: <code><basename>_<solution_name>_<extraction_name>_<quantity>.csv</code>
expression_pattern	Sets the search pattern that specifies which reaction equations are considered for extraction. By default, the search pattern must be given in the glob syntax. To instead enter a regular expression, set <code>pattern_type=regex</code> . You can provide either a pattern or a list of reaction names (parameter <code>reactions</code>). You can specify this parameter only for reaction-dependent quantities (see Table 37). Type: Character Default: none

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define_extraction

Table 36 Parameters of `define_extraction` command for `type=plasma` (Continued)

Parameter	Description
<code>extraction_step</code>	Sets the step interval at which plasma quantities are extracted. You can specify this parameter only for iteration-dependent quantities (see Table 37). You can specify either <code>time_step</code> or <code>extraction_step</code> . Type: Number Default: 1
<code>file</code>	Sets the name of the TDR file. You can specify this parameter only for TDR-exportable quantities (see Table 37) and if <code>output_type=tdr</code> . Type: Character Default: <basename>.tdr
<code>file_update_step</code>	Sets the interval at which output files are written during the simulation. The interval is given in units of the specified <code>time_step</code> or <code>extraction_step</code> , respectively. For example, if <code>file_update_step=1</code> , then files are written at every extraction step. If not specified, then extraction files are written only at the end of the simulation. You can specify this parameter only for iteration-dependent or time-dependent quantities (see Table 37). Type: Number Default: none
<code>log_file_update</code>	Specifies whether to write a short notification in the log output whenever a dataset of the TDR file is updated. Type: Boolean Default: true
<code>max_num_samples</code>	Sets the maximum number of points used for the extraction curves. Type: Number Default: 10000 Range: [2 , ∞)

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Table 36 Parameters of `define_extraction` command for type=plasma (Continued)

Parameter	Description
mode	<p>Controls what happens when the number of extracted time points exceeds the maximum number of samples (specified by <code>max_num_samples</code>). Options are:</p> <ul style="list-style-type: none">• <code>mode=all</code>: Keep the full time range, but resample the datasets to reduce the number of samples.• <code>mode=loop</code>: Keep only the latest time points up to the number specified by <code>max_num_samples</code> and remove all earlier time points. <p>You can specify this parameter only for time-dependent quantities (see Table 37).</p> <p>Type: Character Default: all</p>
name	<p>Sets the name of the extraction. This name is used to reference the extraction in the <code>solve_reactor</code> command (see solve_reactor on page 548).</p> <p>Type: Character Default: none</p>
output_type	<p>Defines the way the extraction data is written. Options are:</p> <ul style="list-style-type: none">• <code>csv</code>: Datasets are written in a tabular format to a CSV file specified by <code>csv_file</code>.• <code>tdr</code>: Datasets are written to a TDR file specified by <code>tdr_file</code>. <p>Type: List Default: <code>tdr</code> if the quantity is exportable to a TDR file (see Table 37), else: <code>csv</code></p>
pattern_type	<p>When using <code>species_pattern</code> or <code>expression_pattern</code> to select the plasma species or reactions, respectively, this parameter sets the type of the pattern. Options are <code>glob</code> and <code>regex</code>.</p> <p>Type: Character Default: <code>glob</code></p>
quantities	<p>Specifies the quantities to be extracted. Table 37 lists the available quantities.</p> <p>If not specified, then all available quantities are extracted.</p> <p>Type: List Default: none</p>

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define_extraction

Table 36 Parameters of `define_extraction` command for type=plasma (Continued)

Parameter	Description
reactions	<p>Specifies the names of the reactions to extract. If not specified, then all reactions are extracted. You can provide either a list of reaction names or a pattern for the reaction equation (parameter <code>expression_pattern</code>). You can specify this parameter only for reaction-dependent quantities (see Table 37).</p> <p>Type: List Default: none</p>
regex_syntax	<p>When using <code>expression_pattern</code> with <code>pattern_type=regex</code> to select the plasma reactions, this parameter defines the syntax of the regular expression. Options are:</p> <ul style="list-style-type: none">• extended• awk• basic• ecma_script• egrep• grep <p>Type: Character Default: extended</p>
sheath_model_type	<p>Sets the type of the sheath model. Depending on the sheath model type, different extraction quantities are available. Options are <code>analytic</code> and <code>circuit</code>.</p> <p>Type: Character Default: none</p>
species	<p>Specifies the names of the species to be considered for extraction. If not specified, then all species are extracted.</p> <p>You can specify this parameter only for species-dependent quantities (see Table 37).</p> <p>Type: List Default: none</p>

Chapter 6: Input Commands

define_extraction

Table 36 Parameters of `define_extraction` command for `type=plasma` (Continued)

Parameter	Description
<code>species_pattern</code>	<p>Sets the search pattern that specifies which species names are considered for extraction. By default, the search pattern must be given in the glob syntax.</p> <p>To instead enter a regular expression, set <code>pattern_type=regex</code>. You can provide either a pattern or a list of species names (parameter <code>species</code>).</p> <p>You can specify this parameter only for species-dependent quantities (see Table 37).</p> <p>Type: Character</p> <p>Default: none</p>
<code>time_step</code>	<p>Sets the time interval at which plasma quantities are extracted.</p> <p>You can specify this parameter only for time-dependent quantities (see Table 37).</p> <p>You can specify either <code>time_step</code> or <code>extraction_step</code>.</p> <p>Type: Number</p> <p>Default: none</p> <p>Unit: s</p>
<code>type</code>	<p>Sets the extraction type. The applicable option is <code>plasma</code>.</p> <p>Type: Character</p> <p>Default: none</p>

Description

For plasma simulations, you can extract different dataset types, for example, time-dependent, iteration-dependent, and energy-dependent curves. [Table 37](#) lists all available extraction quantities with their extraction properties:

- **Time-dependent** quantities can be written at regular time intervals if `file_update_step` is specified. In addition, you can define a `time_step` and the `extraction mode`.
- **Iteration-dependent** quantities can be written at regular iteration intervals if `file_update_step` is specified. In addition, you can define an `extraction_step` and the `extraction mode`.
- Quantities **exportable to TDR files** can be written as a TDR file when `output_type=tdr`.
- Quantities **exportable to CSV files** can be written as a CSV file when `output_type=csv`.

Chapter 6: Input Commands

define_extraction

- For **species-dependent** quantities, you can specify species name filters (see parameters `species` and `species_pattern`).
- For **reaction-dependent** quantities, you can specify the reaction names (parameter `reactions`) or a reaction expression pattern (parameter `expression_pattern`).
- When specifying patterns, you can further choose the `pattern_type` and, if applicable, the `regex_syntax`.

You can define more than one extraction, but each extraction must have a unique name. Finally, you must register a list of the extraction names in the `solve_reactor` command (see [solve_reactor on page 548](#)).

Table 37 Extraction quantities for define_extraction type=plasma command

Model	Quantity	Description	Time dependent	Iteration dependent	Exportable to TDR	Exportable to CSV	Species dependent	Reaction dependent
bulk (global)	electron_energy_distribution	Final energy distribution of the electrons in the bulk			x	x		
bulk (global)	reactions	Number of bulk reaction executions as a function of time	x	x	x	x		x
bulk (global)	residuals	Individual and total convergence residuals as a function of time	x	x	x	x	x	
bulk (global)	species_balance	Time-averaged rates of consumption or production by reactions for each species	x ¹	x		x	x	x
bulk (global)	state	Species densities and electron temperature as a function of time	x	x	x	x	x	
bulk (global)	waveforms	Final density and electron temperature waveforms (only available for pulsed-power models)			x	x	x	
sheath (circuit)	capacitive_displacement_current	Displacement current waveform through the capacitive sheath in the equivalent circuit model		x	x	x		

Chapter 6: Input Commands

define_extraction

Table 37 Extraction quantities for define_extraction type=plasma command (Continued)

Model	Quantity	Description	Time dependent	Iteration dependent	Exportable to TDR	Exportable to CSV	Species dependent	Reaction dependent
sheath (circuit)	electron_current	Electron current waveform through the sheath in the equivalent circuit model (corresponds to the I–V characteristics of a diode)		x	x	x		
sheath (circuit)	energy_distribution	Final energy distributions of the ions and neutrals after passing the sheath layer			x	x	x	
sheath (circuit)	flux	Flux waveform of the particles impinging the electrode			x	x	x	
sheath (circuit)	rf_bias_current	Current waveform applied to the electrode at the RF bias supply		x	x	x		
sheath (circuit)	rf_bias_current_iterations	Amplitudes per frequency of the bias current waveform applied to the electrode at the RF bias supply as a function of the iteration		x	x	x		
sheath (circuit)	rf_bias_power	RF bias power waveform absorbed into the sheath		x	x	x		
sheath (circuit)	rf_bias_power_iterations	The (time-averaged) RF bias power values per frequency as a function of the iteration		x	x	x		
sheath (circuit)	rf_bias_power_residuals	Convergence residual of the RF bias power toward the user-defined target value for each iteration		x	x	x		
sheath (circuit)	rf_bias_voltage	Electric potential waveform between the plasma bulk-sheath-edge and the electrode		x	x	x		

Chapter 6: Input Commands

define_extraction

Table 37 Extraction quantities for define_extraction type=plasma command (Continued)

Model	Quantity	Description	Time dependent	Iteration dependent	Exportable to TDR	Exportable to CSV	Species dependent	Reaction dependent
sheath (circuit)	rf_bias_voltage_iterations	Amplitudes per frequency of the wall potential waveform applied to the electrode at the RF bias supply as a function of the iteration		x	x	x		
sheath (circuit)	sheath_capacitance	Capacitance waveform of the capacitive sheath in the equivalent circuit model		x	x	x		
sheath (circuit)	sheath_width	The distance waveform between the plasma bulk-sheath-edge and the electrode		x	x	x		
sheath (circuit)	total_ion_current	Total ion current waveform through the sheath in the equivalent circuit model		x	x	x		
sheath (circuit)	wall_electric_field_z	Waveform of the vertical component of the electric field at the position of the electrode		x	x	x		
sheath (circuit)	wall_potential	Electric potential waveform between the plasma bulk-sheath-edge and the electrode		x	x	x		
sheath (circuit)	wall_potential_residuals	Convergence residual of the sheath potential drop waveform for each iteration		x	x	x		

- Even if the extracted data is not a function of time, the extraction itself collects time-dependent data. The final extraction data consists of the time-integrated values.

Chapter 6: Input Commands

define_iad

define_iad

This command defines a new ion angular distribution (IAD) that can be used in a flux model. IADs can be defined by either using a tabular format, reading them from a TDR file, or specifying the exponent of an analytic distribution ([Equation 5 on page 49](#)).

Syntax

For built-in models:

```
define_iad exponent=<n> name=<c>  
define_iad file=<c> name=<c> [tdr_geometry=<c>]  
define_iad name=<c> table=<v> [angle_unit=<c>]
```

For RFM models:

```
define_iad exponent=<n> name=<c> species=<c> [energy=<n>]  
define_iad file=<c> name=<c> species=<c> [energy=<n>] [tdr_geometry=<c>]  
define_iad name=<c> species=<c> table=<v> [angle_unit=<c>] [energy=<n>]
```

Then, the defined IAD can be referred to under the name set by the `name` parameter.

Table 38 Parameters of *define_iad* command

Parameter	Description
angle_unit	<p>Sets the unit of the angles listed in the <code>table</code> parameter. Options are:</p> <ul style="list-style-type: none">• deg• rad <p>Type: Character Default: deg</p>
energy	<p>Sets the ion energy for which the angular distribution is defined.</p> <p>Note: When <code>energy=0</code>, the defined distribution is energy independent.</p> <p>Type: Number Default: 0 Range: $[0, \infty[$ Unit: eV</p>

Chapter 6: Input Commands

define_iad

Table 38 Parameters of `define_iad` command (Continued)

Parameter	Description
exponent	Sets the exponent used to characterize the ion angular distribution $\cos^m\theta$. Type: Number Default: none Range: [1, ∞[
file	Sets the name of the TDR file containing an IAD. Type: Character Default: none
name	Sets the name of the IAD. This parameter can be used to reference the IAD in either a <code>define_deposit_machine</code> or a <code>define_etch_machine</code> command. Type: Character Default: none
species	Sets the name of the flux species for which the angular distribution is defined. Type: Character Default: none
table	Sets the tabular format of the IAD (see Tabular Format on page 275 and Examples on page 276). Type: Vector Default: none
tdr_geometry	Sets the name of the geometry to load from a TDR file specified by <code>file</code> . If you omit <code>tdr_geometry</code> , then the geometry to read is specified by the <code>name</code> parameter. Type: Character Default: none

Tabular Format

The format of a table for an IAD is as follows:

- Each line consists of a pair of numbers: The first number represents the angle and the second number represents the value of the flux distribution for this angle.
- The lines are sorted in increasing order by angle.
- The first entry is for angle 0°.
- The last entry is for angle 90° and the flux distribution value is zero.

Chapter 6: Input Commands

define_iad

- Angles must be unique.
- All flux distribution values must be nonnegative and finite.

Note:

A violation of any of these conditions will cause an error.

When using spherical coordinates, the ion flux on a flat unshadowed surface is defined as:

$$\Gamma = \int_0^{2\pi} d\phi \int_0^{\pi/2} \sin\theta \, d\theta \, f(\theta)$$

where $f(\theta)$ is the IAD. Therefore, when using a tabular IAD, the provided data must not contain the factor $\sin\theta$.

The definition of ion distributions is not part of any model. In this way, it is easy to reuse data that has been measured or simulated under certain conditions. In fact, data about many ion fluxes can be stored in a file, which is sourced into the command file when needed.

For example, the following command sets the distribution of the ion flux I according to [Equation 5 on page 49](#) with $m = 100$:

```
define_iad name=my_iad species=I exponent=100
```

The parameter `species` states the name of the flux to which the ion distribution refers.

Sentaurus Topography 3D supports collections of ion distributions, so that data can be reused easily. For example, a collection of ion distributions named `my_iad` is defined with the commands:

```
define_iad name=my_iad species=I1 table=$table1
define_iad name=my_iad species=I2 exponent=1000
define_iad name=my_iad species=I3 table=$table3
```

In this way, the entire collection can be referred to using one name.

Note:

There is no support for energy-dependent flux integration. Therefore, only energy-independent IADs can be used.

Examples

This command loads an IAD with the TDR geometry name `iad_1` from the file `iad.tdr`:

```
define_iad name=iad_1 file=iad.tdr
```

Chapter 6: Input Commands

define_iad

The following commands first define a Tcl variable called `table` that contains a very simple IAD consisting of eleven angles and the corresponding flux distribution values:

```
# Define an IAD table using a Tcl list. First column represents angles
# in degree and second column represents absolute flux values.
set table {
    0.0    1.0
    2.0    0.95
    4.0    0.8
    6.0    0.6
    8.0    0.4
    10.0   0.2
    15.0   0.1
    20.0   0.05
    30.0   0.02
    40.0   0.0
    90.0   0.0
}

# Use the Tcl variable in the definition of the IAD.
define_iad name=my_iad table=$table
```

Note:

The user-defined IADs are normalized internally so that the direct flux on a flat unshadowed surface of the species they refer to equals one.

Chapter 6: Input Commands

define_layout

define_layout

This command reads a GDSII, an OASIS, or a TCAD layout file, which can then be used to create logical masks with the `define_mask` command (see [define_mask on page 281](#)).

Syntax

For GDSII and OASIS layout files:

```
define_layout cell=<c> domain_max=<v> domain_min=<v> \
layer_names=<l> layer_numbers=<l> layout_file=<c> name=<c> \
[domain=<c>] [scale=<n>] [shift_to_origin=<b>] \
[tcad_layout_output_file=<c>]
```

For TCAD layout files:

```
define_layout name=<c> tcad_layout_file=<c> \
[scale=<n>] [shift_to_origin=<b>] [verbose=<b>]
```

Table 39 Parameters of *define_layout* command

Parameter	Description
cell	Sets the name of the layout cell from which a domain is extracted. Type: Character Default: none
domain	Sets the name given to the domain that is extracted from a GDSII or an OASIS layout file. Type: Character Default: SIM3D
domain_max	Sets the 2D maximum point of the layout domain. Type: Vector Default: none Unit: μm
domain_min	Sets the 2D minimum point of the layout domain. Type: Vector Default: none Unit: μm
layer_names	Sets a list of layer names that will be used instead of the layer numbers specified in <code>layer_numbers</code> . The number of entries in both lists must be the same. Type: List Default: none

Chapter 6: Input Commands

define_layout

Table 39 Parameters of *define_layout* command (Continued)

Parameter	Description
layer_numbers	Sets a list of layer numbers that are read from a GDSII or an OASIS layout file. Type: List Default: none
layout_file	Sets the name of a GDSII or an OASIS file from which the layout is read. Type: Character Default: none
name	Sets the name of the layout. Type: Character Default: default_layout
scale	Sets the scaling factor to apply to all layout coordinates. Type: Number Default: 1.0 Range:]0, ∞[
shift_to_origin	Specifies whether to shift the layout, so that the lower-left corner of all domains in the layout shifts to the origin of the simulation coordinate system. Type: Boolean Default: true
tcad_layout_file	Sets the name of the TCAD layout file from which the layout is read. Type: Character Default: none
tcad_layout_output_file	If specified, the layout read from a GDSII or an OASIS file is written to a TCAD layout file with the specified name. Type: Character Default: none
verbose	Specifies whether to output the names of 3D domains and the names of layers in the layout. Type: Boolean Default: false

Chapter 6: Input Commands

define_litho_machine

Examples

Read a layout from a GDSII file:

```
define_layout cell=A10 domain_max={6.5 10.0} domain_min={0 0} \
layer_names={contact} layer_numbers={15:0} \
layout_file=cont.gds name=l
```

define_litho_machine

This command defines a new machine for a lithography process. A lithography machine and its properties are used in a lithography simulation when the name of the machine is specified with the `machine` parameter in the `litho` command.

Note:

A machine defined with the `define_litho_machine` command can be used only to process a 3D structure.

You cannot use this command when you start Sentaurus Topography 3D with a value greater than 1 for the command-line option `--processes` (see [From the Command Line on page 17](#)).

You add properties to the machine by using the `add_litho_command` command (see [add_litho_command on page 176](#)).

Syntax

```
define_litho_machine [name=<c>]
```

Table 40 Parameters of `define_litho_machine` command

Parameter	Description
name	Sets the name of the litho machine that is defined. Type: Character Default: default_machine

Chapter 6: Input Commands

define_mask

define_mask

This command defines a new logical mask.

In contrast to physical masks, logical masks do not have a polarity. They are simply a set of polygons that can be combined by different operations to form new logical masks.

The binary operations and the unary operation `complement`, which are used to form a new mask, can be interpreted as set operations (complement, difference, intersection, symmetric difference, or union) on the polygons in the masks. Except for the operation `difference`, these operations can also be interpreted as simple Boolean operations (*not*, *and*, *xor*, or *or*) where areas covered by polygons have the value *true* and areas that are not covered by polygons have the value *false*.

Note:

To use a logical mask for an etch or a patterning step, you must specify the reticle and resist type with which the logical mask is being used.

Syntax

```
define_mask domain=<c> layer=<c> layout=<c> [name=<c>] [shift=<v>]  
define_mask mask1=<c> mask2=<c> operation=<c> [name=<c>]  
define_mask mask1=<c> operation=complement [name=<c>]  
define_mask mask1=<c> operation=shift shift=<v> [name=<c>]  
define_mask polygon=<v> [domain_max=<v>] [domain_min=<v>] [name=<c>]
```

Table 41 Parameters of *define_mask* command

Parameter	Description
domain	Sets the name of the domain for which a mask is created. Type: Character Default: none
domain_max	Sets the maximum corner point of the mask domain. Sets the upper-left point of a rectangular 2D domain. This domain limits the extent of the inverted mask. It is relevant only if the inverse of the polygonal mask domain is required during an operation involving this mask. Type: Vector Default: {1e3 1e3} Unit: µm

Chapter 6: Input Commands

define_mask

Table 41 Parameters of define_mask command (Continued)

Parameter	Description
domain_min	Sets the minimum corner point of the mask domain. Sets the lower-left point of a rectangular 2D domain. This domain limits the extent of the inverted mask. It is relevant only if the inverse of the polygonal mask domain is required during an operation involving this mask. Type: Vector Default: {-1e3 -1e3} Unit: μm
layer	Sets the name of the layer for which a mask is created. Type: Character Default: none
layout	Sets the name of the layout. Type: Character Default: default_layout
mask1	Sets the name of the input mask for a unary or binary mask operation. Type: Character Default: none
mask2	Sets the name of the input mask for a binary mask operation. Type: Character Default: none
name	Sets the name of the new logical mask. Type: Character Default: default_mask
operation	Sets the operation used to create a new mask from one or two existing masks. Options are: <ul style="list-style-type: none"> • complement • difference • intersection • shift • symmetric_difference • union Type: Character Default: none

Chapter 6: Input Commands

define_mask

Table 41 Parameters of define_mask command (Continued)

Parameter	Description
polygon	Sets the vertices of the polygon defining the mask. The specified vector must be non-empty and contain an even number of elements N . The vector elements are interpreted as the sequence of (x, y) coordinates of the polygon vertices, listed in either a clockwise order or a counterclockwise order. Therefore, the $i \cdot N/2$ -th element contains the x-coordinate of the i -th polygon vertex, and the $(i \cdot N/2 + 1)$ -th element contains the y-coordinate of the i -th polygon vertex. Type: Vector Default: none
shift	Sets the amount by which the output mask is shifted in relation to the input mask. This parameter is required when <code>operation=shift</code> . Type: Vector Default: {0 0} Unit: μm

Limitations

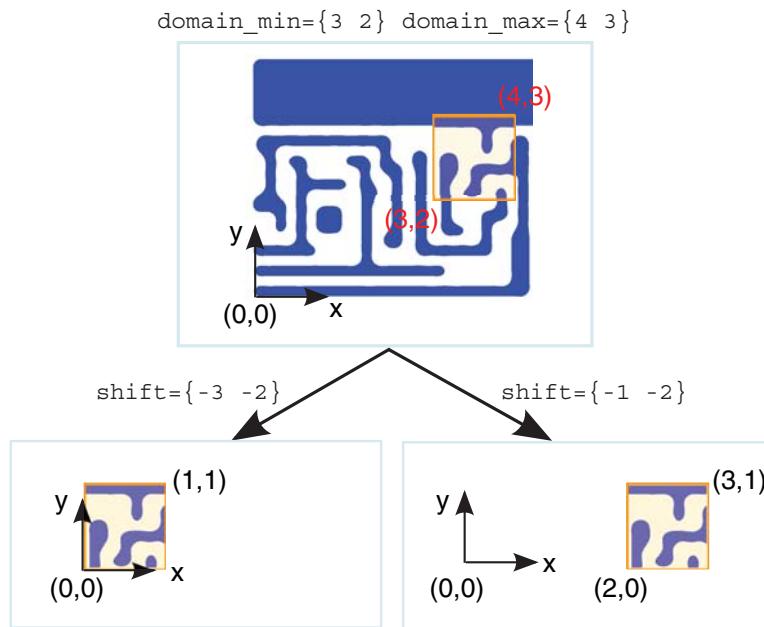
The following limitations apply:

- When performing an operation on two input masks to create a new mask, the domains of the input masks must match.
- Since a domain contains only a small part of the layout, shifting the layout might result in the mask only partially covering the simulation domain, causing unexpected results. Therefore, when analyzing the effects of misaligned layers, it is recommended to define a layout domain that is larger than the simulation domain to ensure that the simulation domain is always fully covered.

Chapter 6: Input Commands

define_mask

Figure 24 Illustration of the relationship of the domain_min, domain_max, and shift parameters



Examples

Define a square mask:

```
define_mask name=m polygon={0 0 1 0 1 1 0 1}
```

Chapter 6: Input Commands

define_material_replacement

define_material_replacement

When running PMC simulations, this command defines a material replacement mapping of a compound material such as SiGe to the constituent PMC species, for example, silicon and germanium.

Syntax

```
define_material_replacement material=<c> name=<c> species=<l> \
    volume_fractions=<l>
```

Mix constant and field-based mole fractions:

```
define_material_replacement constant_species={ cs1 cs2 ... } \
    field_names={ fn1 fn2 ... } field_species={ fs1 fs2 fs3 fs4 ... } \
    volume_fractions={ v1 v2 ... }
```

Table 42 Parameters of *define_material_replacement* command

Parameter	Description
constant_species	<p>Specifies a list of species that are constant in the compound material (material).</p> <p>This parameter is a synonym for the <code>species</code> parameter. It is clearer to specify <code>constant_species</code> and <code>field_species</code>, instead of <code>species</code> and <code>field_species</code>, but both pairs will work.</p> <p>The <code>constant_species</code> list corresponds to the <code>volume_fractions</code> list and must be the same size.</p> <p>Type: Character</p> <p>Default: none</p>
field_names	<p>Specifies a list of fields in the TDR file. Each field sets the mole fraction of two species. The number of <code>field_species</code> should be twice the number of <code>field_names</code>. The values read from the TDR file are restricted to the range 0.0 to 1.0, inclusively. See <i>Description</i> for details.</p> <p>Type: List</p> <p>Default: none (no limit)</p> <p>Unit: μm</p>
field_species	<p>Specifies a list of PMC species corresponding to mole fractions as defined by the TDR fields named in the <code>field_names</code> list. See <i>Description</i> for details.</p> <p>Type: List</p> <p>Default: none (no limit)</p> <p>Unit: μm</p>

Chapter 6: Input Commands

define_material_replacement

Table 42 Parameters of define_material_replacement command (Continued)

Parameter	Description
material	Sets the compound material. Type: Character Default: none
name	Sets the name of the material replacement map. Type: Character Default: none
species	Specifies a list of species corresponding to the compound material defined in the material parameter. Type: List Default: none
volume_fractions	Specifies a list of fractions corresponding to the species defined in the species parameter. The sum of all fractions must be 1.0. Type: List Default: none

Description

The mapping defined by this command can be used in the filter_structure command or the etch command to replace or to *split* the compound material species with its constituents. After the material is split into separate species, you can use different reactions or reaction rates to obtain mole fraction-dependent PMC etching or deposition. Later, the same mapping can be used to restore or to *merge* the original compound material from PMC cells containing the constituent species. The merge operation can be specified with the filter_structure command or can be performed on the fly when saving a boundary file by using the save command.

You can mix constant and field-based mole fractions in the same command specification. The computation of the mole fractions is as follows. Let f_n be the n^{th} field and c_n be the n^{th} constant species given by the volume_fractions parameter. Then, the total of the constant fractions is $\sum_n c_n$.

Now, let R be the fraction available for field-based species, $R = 1 - \sum_n c_n$, and let n_f be the number of field_names.

Chapter 6: Input Commands

define_material_replacement

For each pair p of field_species, f_{2p}, f_{2p+1} , where $0 \leq p < n_f$:

$$\begin{aligned}f_{2p} &= \frac{R}{n_f} \times \text{field_name}[p] \\f_{2p+1} &= \frac{R}{n_f} \times (1 - \text{field_name}[p])\end{aligned}\tag{83}$$

Examples

Convert default_structure from a boundary representation (brep) structure to a PMC structure, and set regions of material SiGe to 40% silicon and 60% germanium:

```
define_material_replacement name=r1 material=SiGe \
    species={Silicon Germanium} volume_fractions={0.4 0.6}
    filter_structure type=convert_to_pmc split_replacements={r1}
```

The sum of the fractions specified in volume_fractions must be 1.0. If not, then fractions are normalized by 1.0/sum-of-all-fractions. If a fraction is modified by more than 1%, then the modified fractions are printed to screen.

Convert default_structure from a brep structure to a PMC structure, and set regions of material AlGaAs to 10% Al, 40% Ga, and 50% As, and proceed to etch the structure with PMC:

```
define_material_replacement name=r2 material=AlGaAs \
    species={ Aluminum Gallium Arsenic } \
    volume_fractions={ 0.1 0.4 0.5 }
    etch split_replacements={ r2 } method=pmc spacing=<n> time=<n>
```

Save structure from previous step, replacing cells of $10\pm5\%$ Al, $40\pm5\%$ Ga, and $50\pm5\%$ As with material AlGaAs:

```
save file=merged.tdr merge_replacements={ r2 } merge_tolerance=0.05
```

Similarly, this command can be used to create a structure merged in memory, which would be available for further processing:

```
filter_structure name=merged merge_replacements={r2} \
    merge_tolerance=0.05
```

Mix constant and field-based mole fractions:

```
define_material_replacement name=sige_mf material=SiliconGermanium \
    field_names={XMoleFraction} field_species={Silicon Germanium}
```

where:

- Total constant species fraction = 0.0
- $R = 1$ and $n_f = 1$

Chapter 6: Input Commands

define_material_replacement

- Germanium = XMoleFraction
- Silicon = $(1 - \text{XMoleFraction})$

```
define_material_replacement name=ingaas_mf material=InGaAs \
    volume_fractions={0.5} constant_species={Arsenic} \
    field_names={XMoleFraction} field_species={Indium Gallium}
```

where:

- Total constant species fraction = 0.5
- $R = 0.5$ and $n_f = 1$
- Arsenic = 0.5
- Indium = $0.5 \times (\text{XMoleFraction})$
- Gallium = $0.5 \times (1 - \text{XMoleFraction})$

```
define_material_replacement name=ingaasp_mf material=InGaAsP \
    field_names={ XMoleFraction YMoleFraction } \
    field_species={ Indium Gallium Arsenic Phosphorus }
```

where:

- Total constant species fraction = 0
- $R = 1$ and $n_f = 2$
- Indium = $1/2 \times (\text{XMoleFraction})$
- Gallium = $1/2 \times (1 - \text{XMoleFraction})$
- Arsenic = $1/2 \times (\text{YMoleFraction})$
- Phosphorus = $1/2 \times (1 - \text{YMoleFraction})$

Chapter 6: Input Commands

define_model

define_model

This command starts the definition of a new RFM model or a reaction model.

Syntax

```
define_model description=<c> name=<c> [type=<c>]
```

Table 43 Parameters of *define_model* command

Parameter	Description
description	Describes the model. Type: Character Default: none
name	Sets the unique name of the model. This name is used to reference the model in all commands for configuring a model and in the <code>define_deposit_machine</code> and <code>define_etch_machine</code> commands, for using the model in a machine. Note: The name must not contain slashes (/). Type: Character Default: none
type	Sets the model type. Options are: <ul style="list-style-type: none">• deposit: Deposition• etch: Etching• etchdepo: Simultaneous etching and deposition If you set this parameter, the new model is assumed to be specified using rate formulas (see add_flux_properties on page 161 , add_formula on page 164 , add_int_parameter on page 166 , add_ion_flux on page 174 , and add_neutral_flux on page 181). If you omit this parameter, the new model is assumed to be a reaction model (see add_reaction on page 182 and add_source_species on page 203). Type: Character Default: none

Chapter 6: Input Commands

define_nad

define_nad

This command defines a new neutral angular distribution (NAD) that can be used in a flux model. NADs can be defined by either using a tabular format, reading them from a TDR file, or specifying the exponent of an analytic distribution (see [Equation 5 on page 49](#)). Then, the defined NAD can be referred to under the name set by the `name` parameter.

Syntax

```
define_nad exponent=<n> name=<c> [energy=<n>] [species=<c>]  
define_nad file=<c> name=<c> [energy=<n>] [species=<c>] \  
[tdr_geometry=<c>]  
define_nad name=<c> table=<v> [angle_unit=<c>] [energy=<n>] \  
[species=<c>]
```

Table 44 Parameters of `define_nad` command

Parameter	Description
angle_unit	Sets the unit of the angles listed in the <code>table</code> parameter. Options are: <ul style="list-style-type: none">• deg• rad Type: Character Default: deg
energy	Sets the neutral energy for which the angular distribution is defined. Note: When <code>energy=0</code> , the defined distribution is energy independent. Type: Number Default: 0 Range: $[0, \infty[$ Unit: eV
exponent	Sets the exponent used to characterize the ion angular distribution $\cos^m\theta$. Type: Number Default: none Range: $[1, \infty[$
file	Sets the name of the TDR file containing a NAD. Type: Character Default: none

Chapter 6: Input Commands

define_nad

Table 44 Parameters of define_nad command (Continued)

Parameter	Description
name	Sets the name of the NAD, which can be used to reference the NAD in either a define_deposit_machine or a define_etch_machine command. Type: Character Default: none
species	Sets the name of the flux species for which the angular distribution is defined. Type: Character Default: neutral
table	Sets the tabular format of the NAD (see Tabular Format on page 275 ; while the content in this section refers to IADs, it also applies to NADs). Type: Vector Default: none
tdr_geometry	Sets the name of the geometry to load from the TDR file specified by file. If you omit tdr_geometry, then the geometry to read is specified by the name parameter. Type: Character Default: none

Description

The definition of neutral distributions is not part of any model. In this way, it is easy to reuse data that has been measured or simulated under certain conditions. In fact, data about many neutral fluxes can be stored in a file, which is sourced into the command file when needed.

For example, the following command sets the distribution of the neutral flux N according to [Equation 5 on page 49](#) with $m=1.5$:

```
define_nad name=my_nad species=N exponent=1.5
```

The parameter species states the name of the flux to which the neutral distribution refers.

Sentaurus Topography 3D supports collections of neutral distributions, so that data can be reused easily. For example, a collection of neutral distributions named my_nad is defined with the commands:

```
define_nad name=my_iad species=N1 table=$table1
define_nad name=my_iad species=N2 exponent=1
define_nad name=my_iad species=N3 table=$table3
```

In this way, the entire collection can be referred to using one name.

Chapter 6: Input Commands

define_nad

Note:

A collection of neutral distributions to be used in a simultaneous etching and deposition machine having `model=etchdepo2` must contain:

- The distribution of the etching neutral flux ($\Gamma_{\text{neutral etch}}$) in [Equation 39 on page 79](#) set with `species=neutral_etch`
- The distribution of the deposition neutral flux ($\Gamma_{\text{neutral depo}}$ in [Equation 39 on page 79](#)) set with `species=neutral`

There is no support for energy-dependent flux integration. Therefore, only energy-independent NADs can be used.

User-defined NADs are normalized internally, so that the direct flux on a flat unshadowed surface of the species they refer to equals one.

Chapter 6: Input Commands

define_pattern_density

define_pattern_density

This command defines a new pattern density object or extends the definition of an existing pattern density object. Each `define_pattern_density` command adds an array of density values that correspond to the cells of a rectangular grid. The position of this grid is specified in coordinates of the simulation domain.

If a pattern density object with the same name already exists, then the new pattern density is added to the already defined pattern density. This behavior allows for the creation of complex pattern density maps by using multiple `define_pattern_density` commands. See [define_pattern_density_model on page 295](#).

Syntax

```
define_pattern_density name=<c> density=<l> point_max=<v> \
    point_min=<v> [n_x=<n>] [n_y=<n>] [type=<c>]
```

Table 45 Parameters of `define_pattern_density` command

Parameter	Description
density	<p>Sets the local pattern densities of the $n_x \times n_y$ grid cells. The value is a list of elements sorted in row-major order from upper-left to bottom-right:</p> $\{ v_{1, n_y} v_{2, n_y} v_{3, n_y} \dots v_{n_x, n_y} \\ \quad \vdots \\ \quad \vdots \\ v_{12} v_{22} v_{32} \dots v_{n_x, 2} \\ v_{11} v_{21} v_{31} \dots v_{n_x, 1} \}$ <p>Type: List Default: none Range: [0, 1]</p>
n_x	<p>Sets the number of grid cells in the x-direction.</p> <p>Type: Number Default: 1 Range: [1, 2147483647]</p>
n_y	<p>Sets the number of grid cells in the y-direction.</p> <p>Type: Number Default: 1 Range: [1, 2147483647]</p>

Chapter 6: Input Commands

define_pattern_density

Table 45 Parameters of define_pattern_density command (Continued)

Parameter	Description
name	Sets the name of the local pattern density object. If a pattern density object with the same name exists already, then the new pattern density is added to the existing pattern density. Type: Character Default: none
point_max	Sets the upper-right corner of the 2D cell grid in coordinates of the simulation domain. Type: Vector Default: none Range: (-∞, ∞) Unit: μm
point_min	Sets the lower-left corner of the 2D cell grid in coordinates of the simulation domain. Type: Vector Default: none Range: (-∞, ∞) Unit: μm
type	Sets the input format of the pattern density. The only option is grid. Type: Character Default: grid

Examples

```
define_pattern_density name=lpd \
    type      = grid \
    n_x       = 2 \
    n_y       = 2 \
    point_min = { 0<um> -1<um> } \
    point_max = { 1<um> 2<um> } \
    density   = { 0.9 0.6 0.8 0.7 }

define_pattern_density name=lpd \
    point_min = { 10 3 } \
    point_max = { 12 5 } \
    density   = 0.5
```

Chapter 6: Input Commands

define_pattern_density_model

define_pattern_density_model

This command defines a new pattern density model that models the pattern density effect observed in semiconductor etching processes. The influence of the pattern density on the etching rate is modeled as:

$$R_{PD} = P(\rho(x, y), \alpha, \beta) \cdot R_{Local} \quad (84)$$

where R_{Local} represents the local etching rate without pattern density effects, and R_{PD} represents the corrected final etching rate. $P(\rho(x, y), \alpha, \beta)$ denotes the rate correction factor that depends on the effective pattern density $\rho(x, y)$ and on the calibration parameters α and β . Here, x and y are coordinates on the wafer surface.

The rate correction factor is given by the following equation, as proposed in [5][6][7][8]:

$$P(\rho(x, y), \alpha, \beta) = e^{-\alpha\rho(x, y)^{\beta}} \quad (85)$$

The effective pattern density $\rho(x, y)$ is constructed by convolution of the *local pattern density* $d(x, y)$, which is defined by the define_pattern_density command (see [define_pattern_density on page 293](#)):

$$\rho(x, y) = (d*f)(x, y) \quad (86)$$

Here, $f(x, y) = \frac{1}{2\pi w^2} \exp\left(-\frac{x^2 + y^2}{2w^2}\right)$ is a Gaussian kernel with range w .

Syntax

```
define_pattern_density_model name=<c> \
    alpha=<n> beta=<n> pattern_density=<c> range=<n> \
    [invert=<b>] [rate_correction_function=<c>] [response_function=<c>]
```

Table 46 Parameters of define_pattern_density_model command

Parameter	Description
alpha	Sets the value of the primary calibration parameter that affects the correction to the pattern density-dependent etching rate. Negative values model a reverse pattern density effect. A value of zero deactivates pattern density-dependent effects. Type: Number Default: none Range: $]-\infty, \infty[$

Chapter 6: Input Commands

define_pattern_density_model

Table 46 Parameters of *define_pattern_density_model* command (Continued)

Parameter	Description
beta	Sets the value of the secondary calibration parameter that affects the correction to the pattern density-dependent etching rate. Type: Number Default: none Range:]0, ∞ [
invert	Specifies whether to invert the local pattern density function, that is, it uses $1 - d(x, y)$ instead of $d(x, y)$. Type: Boolean Default: false
name	Sets the name of the effective pattern density object. Type: Character Default: none
pattern_density	Sets the pattern density object (see define_pattern_density on page 293). Type: Character Default: none
range	Sets the range of influence of a local pattern density impulse. Type: Number Default: none Range:]0, ∞ [Unit: μm
rate_correction_function	Sets the type of the function that corrects the rates as a function of the effective pattern density. The only option is exponential. Type: Character Default: exponential
response_function	Sets the type of the kernel function used in the convolution integral to compute the effective pattern density from the local pattern density. The only option is gaussian. Type: Character Default: gaussian

Chapter 6: Input Commands

define_pattern_density_model

Examples

```
define_pattern_density name=lpd \
    point_min = { 10 3 } \
    point_max = { 12 5 } \
    density    = 0.5

define_pattern_density_model name=pdm \
    pattern_density          = lpd \
    response_function        = gaussian \
    range                    = 1<um> \
    rate_correction_function = exponential \
    alpha                     = 1.1 \
    beta                     = 0.5 \
    invert                   = true
```

Chapter 6: Input Commands

define_plasma_model

define_plasma_model

This command defines a new plasma model. A plasma model consists of a bulk model that describes the physics of the plasma bulk region, and a sheath model that describes the transport of the plasma particles from the plasma bulk region to the structure (see [Chapter 4 on page 99](#)).

In addition, you can define only a plasma bulk model or only a plasma sheath model.

Syntax

A plasma bulk model coupled to a plasma sheath model:

```
define_plasma_model bulk_model_type=<c> name=<c> sheath_model_type=<c>
```

A plasma bulk model only:

```
define_plasma_model bulk_model_type=<c> name=<c>
```

A plasma sheath model only:

```
define_plasma_model name=<c> sheath_model_type=<c>
```

Table 47 Parameters of *define_plasma_model* command

Parameter	Description
bulk_model_type	Sets the bulk model to be used. The only option is <code>global</code> . Type: Character Default: none
name	Sets a unique name for the plasma model. It is used to reference the model in other plasma commands used to configure the model, such as <code>define_reactor</code> (see define_reactor on page 301). Type: Character Default: none
sheath_model_type	Sets the sheath model to be used. Options are: <ul style="list-style-type: none">• <code>analytic</code>• <code>circuit</code> Type: Character Default: none

Examples

```
define_plasma_model name=M bulk_model_type=global
```

```
define_plasma_model name=M sheath_model_type=circuit
```

Chapter 6: Input Commands

define_probability

```
define_plasma_model name=M bulk_model_type=global \
sheath_model_type=circuit
```

define_probability

This command defines a new energy- and angle-dependent probability (hereafter, referred to as the *probability function*).

Syntax

Specify the angle-dependent part of the probability function for a given energy level as a table:

```
define_probability energy=<n> name=<c> table=<v> [angle_unit<c>]
```

or according to the Mizuno model (see [Equation 11 on page 52](#)):

```
define_probability energy=<n> mizuno_k=<n> name=<c>
```

or with an analytic expression:

```
define_probability energy=<n> expression=<c> name=<c>
```

Specify an analytic energy-dependent probability function:

```
define_probability expression=<c> name=<c>
```

Table 48 Parameters of define_probability command

Parameter	Description
angle_unit	Sets the unit of the angles listed in the table parameter. Options are: <ul style="list-style-type: none">• deg• rad Type: Character Default: deg
energy	Sets the energy for which the probability function is defined. Energy-independent probability functions can be specified by setting energy=0. In this case, only one specification for the given name is allowed. Type: Number Default: none Range: [0, ∞[Unit: eV

Chapter 6: Input Commands

define_probability

Table 48 Parameters of define_probability command (Continued)

Parameter	Description
expression	<p>Sets the formula used to calculate the probability function. When you specify expression, the probability function is defined from the user-specified expression, and the energy parameter is optional. For details about energy- and angle-dependent expressions, see Syntax for Expressions on page 139.</p> <p>There are the following cases:</p> <ul style="list-style-type: none"> When energy is not specified, the specified expression defines an energy-dependent probability function that is valid for all energy levels. When energy=0, the specified expression defines an energy-independent probability function. When energy is set to a positive value, the specified expression defines the angle-dependent part of the probability function for the given energy level. <p>Type: Character Default: none</p>
mizuno_k	<p>Sets the species of the parameter k of Equation 11.</p> <p>Type: Number Default: none Range: [0, 1]</p>
name	<p>Sets the name used to refer to the energy- and angle-dependent probability in an add_reaction_properties command.</p> <p>Type: Character Default: none</p>
table	<p>Sets the tabular format of the probability function.</p> <p>When using the parameter table, the same restrictions on the format of the table apply as described in define_iad on page 274, except that the value specified for 90° does not have to be zero. In addition, all of the probability function values must be in the range [0, 1].</p> <p>Type: Vector Default: none</p>

Chapter 6: Input Commands

define_reactor

define_reactor

This command defines the reactor parameters for a plasma model (see [Chapter 4 on page 99](#)).

Syntax

Define a new plasma reactor for a global bulk model (`bulk_model_type=global`):

```
define_reactor name=<c> plasma_model=<c> \
    gas_temperature=<n> height=<n> inlet_gas_flow=<l> \
    (power=<n> | \
     power_period=<n> power_waveform=<c> [num_waveform_samples=<n>]) \
    pressure=<n> radius=<n> type=<c> \
    ([density=<l>] [electron_temperature=<n>] | [solution=<c>] | \
     [solution_file=<c>]) \
    [min_density=<n>] [min_density_relaxation_time=<n>] \
    [min_electron_density=<n>] [min_electron_energy_density=<n>] \
    [outlet_gas_flow=<n>] [power_absorption_coefficient=<n>] \
    [pressure_relaxation_time=<n>]
```

Define a new plasma reactor for an analytic sheath model (`sheath_model_type=analytic`):

```
define_reactor name=<c> plasma_model=<c> \
    gas_temperature=<n> rf_bias_frequency=<n> type=<c> \
    (ac_voltage=<n> dc_voltage=<n> | rf_voltage=<n>) \
    ((density=<l> electron_temperature=<n>) | solution=<c> | \
     solution_file=<c>)
```

Define a new plasma reactor for a circuit sheath model (`sheath_model_type=circuit`):

```
define_reactor name=<c> plasma_model=<c> \
    gas_temperature=<n> height=<n> radius=<n> \
    (rf_bias_frequency=<l> \
     (rf_bias_current=<l> | rf_bias_voltage=<l> | \
      (rf_bias_power=<l> [bias_mode=<c>])) | \
     (bias_current_waveform=<c> bias_current_period=<n> \
      [num_waveform_samples=<n>]) | \
     (wall_potential_waveform=<c> wall_potential_period=<n> \
      [num_waveform_samples=<n>])) \
    ((density=<l> electron_temperature=<n>) | solution=<c> | \
     solution_file=<c>) \
    type=<c>
```

If you couple a bulk model to a sheath model, then provide the union of the parameter sets of the individual models.

Chapter 6: Input Commands

define_reactor

Table 49 Parameters of define_reactor command

Parameter	Description
ac_voltage	<p>Sets the AC sheath voltage of the reactor. Applies only to the analytic sheath model and if rf_voltage is not specified.</p> <p>Type: Number Default: none Range:]0, ∞[Unit: V</p>
bias_current_period	<p>If you specify bias_current_waveform, then you must also define the period of the bias current waveform by using this parameter.</p> <p>Type: Number Default: none Range:]0, ∞[Unit: s</p>
bias_current_waveform	<p>Sets the time-dependent periodic RF current waveform applied to the electrode. This parameter describes the total electric current through the sheath.</p> <p>Note: When using waveform expressions, you must also specify the period of the waveform, using the parameter bias_current_period.</p> <p>You can specify either rf_bias_current or rf_bias_power or bias_current_waveform or wall_potential_waveform. This parameter applies only to the circuit sheath model. For information about the syntax for function expressions, see Syntax for Expressions on page 139.</p> <p>Type: Character Default: Functional expression, depending on time t and evaluating to]0, ∞[Unit: A</p>
bias_mode	<p>If you specify rf_bias_power, then you can also choose the driving mode of the sheath by using this parameter, that is, you can define how the power is fed into the system. Options are current_driven and voltage_driven.</p> <p>Type: Character Default: current_driven</p>

Chapter 6: Input Commands

define_reactor

Table 49 Parameters of define_reactor command (Continued)

Parameter	Description
dc_voltage	<p>Sets the DC sheath voltage of the reactor. Applies only to the analytic sheath model and if rf_voltage is not specified.</p> <p>Type: Number</p> <p>Default: none</p> <p>Range:]0, ∞[</p> <p>Unit: V</p>
density	<p>Sets a list of initial densities for one or more plasma species. The list must be formatted as follows:</p> <pre>{ {species1 value1} {species2 value2} ... }</pre> <p>You can specify either density and electron_temperature, or solution, or solution_file.</p> <p>Type: List</p> <p>Default: Computed automatically from pressure</p> <p>Range: [0, +∞[</p> <p>Unit: m⁻³</p>
electron_temperature	<p>Sets the initial electron temperature.</p> <p>You can specify either density and electron_temperature, or solution, or solution_file.</p> <p>Type: Number</p> <p>Default: 2</p> <p>Range:]0, ∞[</p> <p>Unit: eV</p>
gas_temperature	<p>Sets the temperature of the neutral gas.</p> <p>Type: Number</p> <p>Default: none</p> <p>Range:]0, ∞[</p> <p>Unit: K</p>
height	<p>Sets the effective height of the plasma bulk (see parameter <i>L_{bulk}</i>, Equation 49).</p> <p>Type: Number</p> <p>Default: none</p> <p>Range:]0, ∞[</p> <p>Unit: m</p>

Chapter 6: Input Commands

`define_reactor`

Table 49 Parameters of `define_reactor` command (Continued)

Parameter	Description
<code>inlet_gas_flow</code>	Sets a list of inlet gas flow rates for one or more plasma species. The list must be formatted as follows: $\{ \{ \text{species1} \text{ value1} \} \{ \text{species2} \text{ value2} \} \dots \}$ Type: List Default: 0 Range: $[0, +\infty[$ Unit: sccm
<code>min_density</code>	Sets the numeric minimal density for every species. Type: Number Default: 1 Range: $[0, +\infty[$ Unit: m^{-3}
<code>min_density_relaxation_time</code>	Sets the numeric relaxation time to the minimum density. Type: Number Default: 10^{-6} Range: $]0, +\infty[$ Unit: s
<code>min_electron_density</code>	Sets the numeric minimal density of electrons. Type: Number Default: 10^{15} Range: $[0, +\infty[$ Unit: m^{-3}
<code>min_electron_energy_density</code>	Sets the numeric minimal energy density of electrons. Type: Number Default: 1 Range: $[0, +\infty[$ Unit: eV m^{-3}
<code>name</code>	Sets the name of the reactor. This name is used to refer to the reactor in other commands, such as <code>solve_reactor</code> (see solve_reactor on page 548). Type: Character Default: none

Chapter 6: Input Commands

define_reactor

Table 49 Parameters of define_reactor command (Continued)

Parameter	Description
num_waveform_samples	<p>Sets the number of samples used to resolve the specified waveform expressions.</p> <p>You can specify this parameter only if <code>bias_current_waveform</code>, <code>power_waveform</code>, or <code>wall_potential_waveform</code> is specified.</p> <p>Type: Number Default: 100 Range: [2, +∞[</p>
outlet_gas_flow	<p>Sets the initial outlet gas flow rate.</p> <p>The outlet gas flow changes during the simulation to reach the given pressure value (parameter <code>pressure</code>).</p> <p>Type: Number Default: 0 Range: [0, +∞[Unit: sccm</p>
plasma_model	<p>Sets the name of the plasma model, which must have been already defined by the <code>define_plasma_model</code> command (see define_plasma_model on page 298).</p> <p>Type: Character Default: none</p>
power	<p>Sets the RF power applied to the reactor.</p> <p>The power absorbed by the electrons and ions in the plasma bulk is the product of the parameters <code>power</code> and <code>power_absorption_coefficient</code>.</p> <p>You can specify either <code>power</code> or <code>power_waveform</code>.</p> <p>Type: Number Default: none Range:]0, ∞[Unit: W</p>
power_absorption_coefficient	<p>Sets the fraction of the applied RF power absorbed by the electrons and ions in the plasma bulk.</p> <p>Type: Number Default: 1 Range:]0, 1]</p>

Chapter 6: Input Commands

define_reactor

Table 49 Parameters of define_reactor command (Continued)

Parameter	Description
power_period	If you specify power_waveform, then you must also define the period of the power waveform by using this parameter. Type: Number Default: none Range:]0, ∞[Unit: s
power_waveform	Sets the time-dependent periodic RF power waveform applied to the reactor. Note: When using waveform expressions, you must also specify the period of the power waveform, by using the parameter power_period. You can specify either power or power_waveform. For information about the syntax for function expressions, see Syntax for Expressions on page 139 . Type: Character Default: Functional expression, depending on time t and evaluating to]0, ∞[Unit: W
pressure	Sets the pressure inside the reactor. The pressure remains constant during the simulation by a pressure controller (see the pressure_relaxation_time parameter). Type: Number Default: none Range:]0, ∞[Unit: Pa
pressure_relaxation_time	Sets the characteristic relaxation time of the pressure controller. The pressure controller calibrates the outlet gas flow to match the target pressure given by the pressure parameter. Type: Number Default: 10^{-6} Range:]0, ∞[Unit: s

Chapter 6: Input Commands

define_reactor

Table 49 Parameters of define_reactor command (Continued)

Parameter	Description
radius	Sets the effective radius of the plasma bulk (see parameter R_{bulk} , Equation 49). Type: Number Default: none Range:]0, ∞ [Unit: m
reactor	Sets the name of another plasma reactor that will be used as a template for creating the new reactor. All parameters of this reactor are initialized with the values of the template reactor. You can also change some values by explicitly specifying the corresponding parameters. Type: Character Default: none
rf_bias_current	Specifies the amplitudes $\{I_i\}$ of the sinusoidal current applied at the electrode: $I(t) = \sum_i I_i \sin(2\pi f_i t)$ This parameter applies only to the circuit sheath model. Type: List Default: none Range: Each bias current must be in the range]0, ∞ [Unit: A
rf_bias_frequency	Specifies the bias frequencies $\{f_i\}$ of the sinusoidal current or voltage applied at the electrode (see parameters <code>rf_bias_current</code> and <code>rf_bias_voltage</code> for details). This parameter applies only to the circuit sheath model. Type: List Default: none Range: Each bias frequency must be in the range]0, ∞ [Unit: Hz

Chapter 6: Input Commands

define_reactor

Table 49 Parameters of define_reactor command (Continued)

Parameter	Description
rf_bias_power	<p>Specifies the power $\{P_i\}$ absorbed into the sheath per frequency.</p> <p>For bias_mode=current_driven:</p> $P_i = -\frac{1}{\tau} \int_0^{\tau} I_i \sin(2\pi f_i t) \cdot V_W(t) dt$ <p>For bias_mode=voltage_driven:</p> $P_i = -\frac{1}{\tau} \int_0^{\tau} I(t) \cdot V_i \sin(2\pi f_i t) dt$ <p>This parameter applies only to the circuit sheath model.</p> <p>Type: List</p> <p>Default: none</p> <p>Range: Each bias power must be in the range]0, ∞[</p> <p>Unit: W</p>
rf_bias_voltage	<p>Specifies the amplitudes $\{V_i\}$ of the sinusoidal voltage applied at the electrode:</p> $V(t) = V_{DC} + \sum_i V_i \sin(2\pi f_i t)$ <p>Note that V_{DC} is computed automatically in a self-consistent way.</p> <p>This parameter applies only to the circuit sheath model.</p> <p>Type: List</p> <p>Default: none</p> <p>Range: Each voltage must be in the range]0, ∞[</p> <p>Unit: V</p>
rf_voltage	<p>Sets the amplitude of the RF voltage applied to the reactor. Applies only to the analytic sheath model.</p> <p>Type: Number</p> <p>Default: none</p> <p>Range:]0, ∞[</p> <p>Unit: V</p>

Chapter 6: Input Commands

define_reactor

Table 49 Parameters of *define_reactor* command (Continued)

Parameter	Description
solution	Sets the name of the plasma solution, which is used to initialize the state of the reactor (= initial densities and electron temperature). The solution name is specified in the command <code>solve_reactor</code> (see solve_reactor on page 548). You can specify either <code>density</code> and <code>electron_temperature</code> , or <code>solution</code> , or <code>solution_file</code> . Type: Character Default: none
solution_file	Sets the name of the file containing the plasma solution, which is used to initialize the state of the reactor (= initial densities and electron temperature). You can specify either <code>density</code> and <code>electron_temperature</code> , or <code>solution</code> or <code>solution_file</code> . Type: Character Default: none
type	Sets the type of the plasma reactor. Options are: <ul style="list-style-type: none">• <code>ccp</code>• <code>icp</code> Type: Character Default: none
wall_potential_period	If you specify <code>wall_potential_waveform</code> , then you must also define the period of the wall potential waveform by using this parameter. Type: Number Default: none Range:]0, ∞[Unit: s

Chapter 6: Input Commands

define_reactor

Table 49 Parameters of define_reactor command (Continued)

Parameter	Description
wall_potential_waveform	<p>Sets the time-dependent periodic RF voltage waveform applied to the electrode. The voltage describes the potential drop across the sheath and is defined as the difference between the plasma potential and the electrode potential.</p> <p>Note: When using waveform expressions, you must also specify the period of the waveform, using the parameter <code>wall_potential_period</code>.</p> <p>You can specify either <code>rf_bias_current</code> or <code>rf_bias_power</code> or <code>bias_current_waveform</code> or <code>wall_potential_waveform</code>. This parameter applies only to the circuit sheath model. For information about the syntax for function expressions, see Syntax for Expressions on page 139.</p> <p>Type: Character Default: Functional expression, depending on time t and evaluating to $]-\infty, +\infty[$ The time-averaged wall potential (DC part) must be negative Unit: V</p>

Note:

Gas flows are typically specified in units of standard cubic centimeters per minute (sccm). The model implicitly converts sccm to SI units, which is given by:

$$1 \text{ sccm} = \frac{p_0}{k_B T_0} \frac{\text{cm}^3}{\text{min}} = 4.4194 \cdot 10^{17} \frac{\text{particles}}{\text{s}}$$

for $p_0 = 10^5 \text{ Pa}$ and $T_0 = 273.15 \text{ K}$ (according to the IUPAC; see [STP on page 621](#)).

Examples

```
define_reactor name=R plasma_model=M type=icp radius=15<cm> \
height=7.5<cm> gas_temperature=305<K> pressure=10<mTorr> \
rf_bias_frequency=1<MHz> rf_bias_power=20<W> power=800<W> \
density={{Ar 1e16<m^-3>} {Ar* 1e14<m^-3>}} \
inlet_gas_flow={{Ar 20<sccm>} {Ar* 0.1<sccm>}} \
solve_reactor name=soll reactor=R
```

Chapter 6: Input Commands

define_reflection

define_reflection

This command specifies the properties of a new reflection function that depends on the ion species, the ion energy, and the surface material.

This reflection function can be used in RFM models that take reflection into account.

Syntax

```
define_reflection energy=<n> material=<c> name=<c> species=<c> \
    table=<v> [angle_unit=<c>]

define_reflection energy=<n> material=<c> name=<c> species=<c> \
    reflection=<n>
```

Table 50 Parameters of *define_reflection* command

Parameter	Description
angle_unit	Sets the unit of the angles listed in the table parameter. Options are: <ul style="list-style-type: none">• deg• rad Type: Character Default: deg
energy	Sets the energy for which the reflection function is defined. Energy-independent reflection functions can be specified by setting energy=0. In this case, only one specification for each combination of ion species and surface material is allowed. Type: Number Default: none Range: [0, ∞[Unit: eV
material	Sets the name of the surface material for which the reflection function is defined. Type: Character Default: none
name	Sets the name used to reference the reflection function in a define_deposit_machine or define_etch_machine command. Type: Character Default: none

Chapter 6: Input Commands

define_reflection

Table 50 Parameters of define_reflection command (Continued)

Parameter	Description
reflection	Sets the reflection parameter used to evaluate the reflection probability according to Equation 11 . Type: Number Default: none Range: [0, 1]
species	Sets the name of the flux species for which the reflection function is defined. Type: Character Default: none
table	Sets the tabular format of the reflection function. When using the parameter <code>table</code> , the same restrictions on the format of the table apply as described in define_iad on page 274 , except that the value specified for 90° does not have to be zero. In addition, all reflection probability values must be in the range [0, 1]. Type: Vector Default: none

Description

For energy-dependent reflection functions, for each combination of ion species and surface material, the properties of the reflection function for at least two different energy levels must be specified.

For energy values that have not been specified, the value of the reflection function is calculated by linearly interpolating the values of the parameter `reflection` for the analytic reflection function or the specified values for the tabular reflection functions.

Sentaurus Topography 3D supports collections of reflection functions, as shown by the following commands, which define a collection of energy-independent reflection functions called `my_reflection` for flux `I` and several target materials:

```
define_reflection name=my_reflection species=I energy=0 \
    material=Silicon reflection=0.4

define_reflection name=my_reflection species=I energy=0 \
    material=Oxide reflection=0.1

define_reflection name=my_reflection species=I energy=0 \
    material=Nitride table=$reflection_table

define_reflection name=my_reflection species=I energy=0
    material=Photoresist reflection=0.9
```

Chapter 6: Input Commands

define_shape

Note:

There is no support for energy-dependent flux integration. Therefore, only energy-independent reflection functions can be used.

define_shape

This command defines a new shape for a geometric etch or deposit step.

Syntax

Cone (3D):

```
define_shape type=cylinder name=<c> center1=<v> center2=<v> \
    radius1=<n> radius2=<n> \
    [refinement=<n>] [<transformation_options>]
```

Cone (3D) with circular cross-section:

```
define_shape type=cylinder name=<c> center1=<v> center2=<v> \
    radius1=<n> radius2=<n> \
    [refinement=<n>] [rotation=<n>] [<transformation_options>]
```

Cone (3D) with elliptic cross-section (see [Figure 25](#)):

```
define_shape type=cylinder name=<c> \
    center1=<v> center2=<v> \
    radius1_a=<n> radius1_b=<n> radius2_a=<n> [radius2_b=<n>] \
    [elliptic_exponent=<n> | (elliptic_exponent1=<n> \
    elliptic_exponent2=<n>)] \
    [refinement=<n>] \
    [rotation=<n> | (rotation1=<n> rotation2=<n>)] \
    [<transformation_options>]
```

Cylinder (3D) with circular cross-section:

```
define_shape type=cylinder name=<c> center1=<v> center2=<v> \
    radius=<n> \
    [refinement=<n>] [rotation=<n>] [<transformation_options>]
```

Cylinder (3D) with elliptic cross-section:

```
define_shape type=cylinder name=<c> center1=<v> center2=<v> \
    radius_a=<n> radius_b=<n> \
    [elliptic_exponent=<n>] [refinement=<n>] [rotation=<n>] \
    [<transformation_options>]
```

Chapter 6: Input Commands

define_shape

Cuboid (3D):

```
define_shape type=cube name=<c> point_max=<v> point_min=<v> \
([scale_bottom=<n>] | [scale_bottom_x=<n>] [scale_bottom_y=<n>]) \
([scale_top=<n>] | [scale_top_x=<n>] [scale_top_y=<n>]) \
[<transformation_options>]
```

Ellipsoid (3D):

```
define_shape type=ellipsoid name=<c> center=<v> radius_a=<n> \
radius_b=<n> radius_c=<n> \
[refinement=<n>] [<transformation_options>]
```

Sphere (3D):

```
define_shape type=sphere name=<c> center=<v> radius=<n> \
[refinement=<n>] [<transformation_options>]
```

Extruded mask (3D):

```
define_shape type=mask mask=<c> profile=<v> name=<c> \
[invert_mask=<b>] [<transformation_options>]

define_shape type=mask mask=<c> taper_angles=<v> z_coordinates=<v> \
name=<c> [invert_mask=<b>] [<transformation_options>]
```

Circle (2D):

```
define_shape type=circle center=<v> radius=<n> [refinement=<n>]
```

Rectangle (2D):

```
define_shape type=rectangle point_max=<v> point_min=<v> \
[scale_bottom=<n>] [scale_top=<n>]
```

Asymmetric hole (3D):

```
define_shape type=asymmetric_hole name=<c> center=<v> \
profile1=<l> profile2=<l> \
[rotation=<n>] [refinement=<n>] [<transformation_options>]
```

An asymmetric hole is a generalized 3D vertical cylinder with an arbitrary vertical profile, specified by two vertical surface lines `profile1` and `profile2` (see [Figure 26 on page 329](#)). At each height z , the contour of the xy cross-section of the asymmetric hole is a circle.

Here, `center` is a 2D point defining the xy position of the vertical reference axis of the hole. The parameters `profile1` and `profile2` are the left and right surface lines of the hole, respectively, given as a list of lateral offsets as a function of z . By default, the left and right surface lines are located along the x -direction from the given reference axis. To measure the surface lines in another direction from the reference axis, you can use the `rotation` parameter, which defines the measurement direction of the offsets in the xy plane

Chapter 6: Input Commands

define_shape

(rotation=0: along the x-axis (default), rotation=90: along the y-axis, rotation=180: along the -x-axis, and so on).

Stacked cylinder (3D):

```
define_shape type=stacked_cylinder name=<c> center_list=<v> \
  (radius_list=<v> | (radius_a_list=<v> radius_b_list=<v>)) \
  [elliptic_exponent_list=<v>] [refinement=<n>] [rotation_list=<v>] \
  [<transformation_options>]
```

A stacked cylinder consists of a sequence of 3D cylinders or cones, stacked on each other. Therefore, type=stacked_cylinder is a generalization of type=cylinder for multiple cylinders. The vertical stack of cylinders is specified by a sequence of 3D cylinder axis points, given by the center_list parameter. For each axis point, you can specify the radius of the cylinder, measured in the xy plane through that axis point. Use the parameter radius_list to define circular cross sections, or the parameters radius_a_list, radius_b_list, rotation_list, or elliptic_exponent_list to define elliptic cross sections.

Table 51 Parameters of *define_shape* command

Parameter	Description
center	Sets the center point of a sphere or circle. For an asymmetric hole, it sets the xy position of the vertical reference axis of the hole. The format is {x y}. Type: Vector Default: none Range:]-∞, +∞[Unit: μm
center_list	Specifies a flat list of 3D cylinder axis points along the z-axis. The format is {x1 y1 z1 x2 y2 z2 ...}.
	Note: The z-values must be either increasing monotonically or decreasing monotonically. Type: List Default: none Range:]-∞, +∞[Unit: μm
center1	Sets the first axis point of a cylinder. Type: Vector Default: none Unit: μm

Chapter 6: Input Commands

`define_shape`

Table 51 Parameters of `define_shape` command (Continued)

Parameter	Description
<code>center2</code>	Sets the second axis point of a cylinder. Type: Vector Default: none Unit: μm
<code>elliptic_exponent</code>	Sets the exponent p in the equation defining the (super-)ellipse curve: $\left(\frac{ x }{r_1}\right)^p + \left(\frac{ y }{r_2}\right)^p = 1$ Type: Number Default: 2 Range: $[0, \infty]$
<code>elliptic_exponent_list</code>	Specifies a list of elliptic exponents p of the elliptical cross-sections along the z-axis (one value for each axis point in <code>center_list</code>). Type: List Default: 2 Range: $[0, \infty]$
<code>elliptic_exponent1</code>	Sets the exponent p for the ellipse with the center at <code>center1</code> . Type: Number Default: 2 Range: $[0, \infty]$
<code>elliptic_exponent2</code>	Sets the exponent p for the ellipse with the center at <code>center2</code> . Type: Number Default: 2 Range: $[0, \infty]$
<code>invert_mask</code>	Specifies whether to use the inverted mask instead of the regular mask. Type: Boolean Default: false
<code>mask</code>	Sets the name of the mask defined in a <code>define_mask</code> command. Type: Character Default: none

Chapter 6: Input Commands

define_shape

Table 51 Parameters of define_shape command (Continued)

Parameter	Description
name	Sets the unique name of the shape. Type: Character Default: none
point_max	Sets the maximum corner point of a cube or rectangle. Type: Vector Default: none Unit: μm
point_min	Sets the minimum corner point of a cube or rectangle. Type: Vector Default: none Unit: μm
profile	Specifies a list of pairs of lateral coordinates and z-coordinates, for example, {11 z1 12 z2}. The lateral coordinates are measured relative to the edge of the 2D mask. Positive lateral coordinates mean the mask is slanted outside, and negative values slant the mask inside. The coordinate pairs are ordered either in ascending or descending z order. Type: Vector Default: none Unit: μm
profile1	Defines the (left) surface line of a hole. You must specify the horizontal distance of the surface to the reference axis of the hole as a function of z. The z-coordinates must be sorted in either increasing order or decreasing order. The first and last z-coordinates in profile1 and profile2 must coincide. The format is {11 z1 12 z2 ...}.
	Type: List Default: none Range:] $-\infty$, $+\infty$ [Unit: μm

Chapter 6: Input Commands

define_shape

Table 51 Parameters of define_shape command (Continued)

Parameter	Description
profile2	<p>Defines the (right) surface line of a hole, opposite to the surface line given in <code>profile1</code>. You must specify the horizontal distance of the surface to the reference axis of the hole as a function of z. The z-coordinates must be sorted in either increasing order or decreasing order.</p> <p>The first and last z-coordinates in <code>profile1</code> and <code>profile2</code> must coincide. The format is {11 z1 12 z2 ...}.</p> <p>Type: List Default: none Range:]-∞, +∞[Unit: μm</p>
radius	<p>Sets the radius of a circle, a sphere, or a cylinder base circle.</p> <p>Type: Number Default: none Range: [0, ∞[Unit: μm</p>
radius_a	<p>Sets the main axis length in the x-direction for an elliptic cylinder or ellipsoid.</p> <p>Type: Number Default: none Range: [0, ∞[Unit: μm</p>
radius_a_list	<p>Specifies a list of main axis lengths in the x-direction of the elliptical cross-sections along the z-axis (one value for each axis point in <code>center_list</code>).</p> <p>Type: List Default: none Range: [0, ∞[Unit: μm</p>
radius_b	<p>Sets the main axis length in the y-direction for an elliptic cylinder or ellipsoid.</p> <p>Type: Number Default: none Range: [0, ∞[Unit: μm</p>

Chapter 6: Input Commands

define_shape

Table 51 Parameters of *define_shape* command (Continued)

Parameter	Description
radius_b_list	Specifies a list of main axis lengths in the x-direction of the elliptical cross-sections along the z-axis (one value for each axis point in center_list). Type: List Default: none Range: [0, ∞[Unit: μm
radius_c	Sets the main axis length in the z-direction for an ellipsoid. Type: Number Default: none Range: [0, ∞[Unit: μm
radius1	Sets the radius of the circle with the center at center1 of a truncated cone. Type: Number Default: none Range: [0, ∞[Unit: μm
radius1_a	Sets the main axis length in the x-direction of the ellipse with the center at center1 of an elliptic cylinder. Type: Number Default: none Range: [0, ∞[Unit: μm
radius1_b	Sets the main axis length in the y-direction of the ellipse with the center at center1 of an elliptic cylinder. Type: Number Default: none Range: [0, ∞[Unit: μm

Chapter 6: Input Commands

define_shape

Table 51 Parameters of define_shape command (Continued)

Parameter	Description
radius2	Sets the radius of the circle with the center at <code>center2</code> of a truncated cone. Type: Number Default: none Range: $[0, \infty[$ Unit: μm
radius2_a	Sets the main axis length in the x-direction of the ellipse with the center at <code>center2</code> of an elliptic cylinder. Type: Number Default: none Range: $[0, \infty[$ Unit: μm
radius2_b	Sets the main axis length in the y-direction of the ellipse with the center at <code>center2</code> of an elliptic cylinder. Type: Number Default: none Range: $[0, \infty[$ Unit: μm
refinement	Sets the refinement as follows: <ul style="list-style-type: none"> • If a circle, this is the number of circle vertices. • If a cylinder, this is the number of base circle points of the cylinder. • If a sphere, this is the number of icosahedron faces: $20 \cdot 4^{\text{refinement}}$. • If an asymmetric hole, this is the number of circle points at each orthogonal cross-section to the hole axis. Type: Number Default: 20 (circle), 20 (cylinder), 2 (sphere), 20 (asymmetric hole) Range: $[1, \infty[$

Chapter 6: Input Commands

define_shape

Table 51 Parameters of define_shape command (Continued)

Parameter	Description
rotation	Sets the angle by which a cone or cylinder is rotated about its axis. For an asymmetric hole, it defines the measurement direction of the distance between the surface line and the vertical reference axis. For example, if rotation=0, the lateral offsets given in profile1 and profile2 are measured in the x-direction. If rotation=90, the lateral offsets are measured in the y-direction, and so on. Type: Number Default: 0 Range: [-180, 180] Unit: degree
rotation_list	Specifies a list of rotation angles of the elliptical cross-sections along the z-axis (one value for each axis point in center_list). Type: List Default: 0 Range: [-180, 180] Unit: degree
rotation1	Sets the angle by which the ellipse with the center at center1 is rotated about the axis through center1 and center2. Type: Number Default: 0 Range: [-180, 180] Unit: degree
rotation2	Sets the angle by which the ellipse with the center at center2 is rotated about the axis through center1 and center2. Type: Number Default: 0 Range: [-180, 180] Unit: degree
scale_bottom	Sets the scale factor for the bottom face or edge of the initial cube or rectangle. A truncated pyramid or a symmetric trapezoid is created instead of a cube or a rectangle, respectively. Type: Number Default: 1 Range: [0, ∞[

Chapter 6: Input Commands

define_shape

Table 51 Parameters of define_shape command (Continued)

Parameter	Description
scale_bottom_x	Sets the scale factor for the two sides parallel to the x-axis of the bottom face of a cube. Type: Number Default: 1 Range: [0 , ∞[
scale_bottom_y	Sets the scale factor for the two sides parallel to the y-axis of the bottom face of a cube. Type: Number Default: 1 Range: [0 , ∞[
scale_top	Sets the scale factor for the top face or edge of the initial cube or rectangle. A truncated pyramid or a symmetric trapezoid is created instead of a cube or a rectangle, respectively. Type: Number Default: 1 Range: [0 , ∞[
scale_top_x	Sets the scale factor for the two sides parallel to the x-axis of the top face of a cube. Type: Number Default: 1 Range: [0 , ∞[
scale_top_y	Sets the scale factor for the two sides parallel to the y-axis of the top face of a cube. Type: Number Default: 1 Range: [0 , ∞[
taper_angles	Specifies a list of taper angles to be specified in combination with z_coordinates. The number of taper angles must match the number of intervals. Therefore, this vector has one element less than z_coordinates. Type: Vector Default: none Range: Each vector element must be in the range [-89 , 89] Unit: degree

Chapter 6: Input Commands

define_shape

Table 51 Parameters of *define_shape* command (Continued)

Parameter	Description
<transformation_options>	Specifies a set of parameters with which to transform the shape after creation (see <i>Shape Transformations: <transformation_options></i>). Type: Character Default: none
type	Sets the shape to be defined. Options are: <ul style="list-style-type: none">• asymmetric_hole• circle• cube• cylinder• ellipsoid• mask• rectangle• sphere• stacked_cylinder Type: Character Default: none
z_coordinates	Specifies a list of z-coordinates to be specified in combination with taper_angles. The slant of the intervals is specified with taper_angles; therefore, z_coordinates requires one element more than taper_angles. Type: Vector Default: none Unit: μm

Shape Transformations: <transformation_options>

Depending on the required transformation, you need to specify the following parameters:

- For an Euler rotation: alpha=<n> beta=<n> gamma=<n>
- For a rotation around a specified axis, one of the following:
 - axis=<c> axis_rotation=<n> point=<v>
 - axis_rotation=<n> direction=<v> point=<v>
 - axis_rotation=<n> point1=<v> point2=<v>

Chapter 6: Input Commands

define_shape

- For shearing or tilting: shear_fix_axis=<n> shear_fix_position=<n>
shear_rotation=<n> shear_tilt=<n>

[Table 52](#) lists the parameters specifically for transforming shapes.

Table 52 Parameters for shape transformations

Parameter	Description
alpha	Sets the first Euler angle for rotating an ellipsoid. Type: Number Default: 0 Range: [-180, 180] Unit: degree
axis	Sets the rotation direction to one of the coordinate axes. It depends on the parameter point. Options are: <ul style="list-style-type: none">• x• y• z Type: Character Default: none
axis_rotation	Sets the angle by which the shape is rotated around a specified axis. Type: Number Default: 0 Range: [-180, 180] Unit: degree
beta	Sets the second Euler angle for rotating an ellipsoid. Type: Number Default: 0 Range: [-180, 180] Unit: degree
direction	Sets the direction of the rotation axis. It depends on the parameter point. Type: Vector Default: none Unit: μm
gamma	Sets the third Euler angle for rotating an ellipsoid. Type: Number Default: 0 Range: [-180, 180] Unit: degree

Chapter 6: Input Commands

define_shape

Table 52 Parameters for shape transformations (Continued)

Parameter	Description
point	Sets a point along the rotation axis. It depends on the parameter axis_rotation. Type: Vector Default: none Unit: µm
point1	Sets the first point of the rotation axis. It depends on the parameter axis_rotation. Type: Vector Default: none Unit: µm
point2	Sets the second point of the rotation axis. It depends on the parameter point1. Type: Vector Default: none Unit: µm
shear_rotation	Sets the angle of the shear direction. By default, the shear direction is: <ul style="list-style-type: none"> • x if shear_fix_axis=z • y if shear_fix_axis=x • z if shear_fix_axis=y Then, the direction is rotated around the shear_fix_axis by the shear_rotation angle to calculate the shearing direction. Type: Number Default: 0 Range: [-180, 180] Unit: degree
shear_fix_position	Sets the distance of the fixed plane to the coordinate root. The distance is measured in the direction given by shear_fix_axis. If this parameter is not set, then it is set internally to the highest point of the structure. This parameter depends on the shear_tilt parameter. Type: Number Default: none Unit: µm

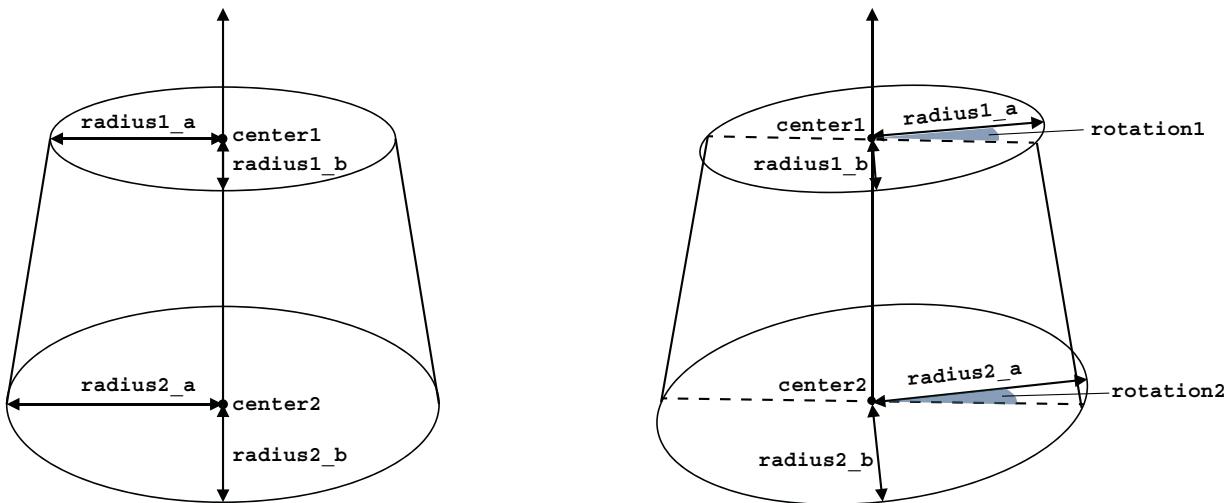
Chapter 6: Input Commands

define_shape

Table 52 Parameters for shape transformations (Continued)

Parameter	Description
shear_fix_axis	<p>Sets the axis that defines the fixed plane for the shearing operation. Options are:</p> <ul style="list-style-type: none"> • x • y • z <p>This parameter depends on the shear_tilt parameter.</p> <p>Type: String Default: z</p>
shear_tilt	<p>Sets the angle by which the shape is tilted.</p> <p>Type: Number Default: 0 Range: [-89, 89] Unit: degree</p>

Figure 25 (Left) Three-dimensional cone with elliptic cross section and (right) same cone with rotation or twisting



Examples

Define a 2D circle with center {0.0 0.0}, radius 1.0 µm, and name circle_1:

```
define_shape type=circle name=circle_1 center={0.0 0.0} radius=1.0
```

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define_shape

Define a 2D rectangle with corners {0.0 0.0} {1.0 1.0} and the name r_1:

```
define_shape type=rectangle name=r_1 point_max={1.0 1.0} \
point_min={0.0 0.0}
```

Define a cuboid with bounding points {0.25 0.25 0.25}, {0.75 0.75 1.0} and with the name cube_1 (the cuboid can be used in a subsequent etching or deposition step):

```
define_shape type=cube name=cube_1 point_max={0.75 0.75 1.0} \
point_min={0.25 0.25 0.25}
```

Define a cylinder with an axis of {0.0 0.0 0.0}, {0.0 0.0 1.0} parallel to the z-axis, with a radius of 0.25 µm and the name cylinder_1 (the cylinder can be used in a subsequent etching or deposition step):

```
define_shape type=cylinder name=cylinder_1 \
center1={0.0 0.0 0.0} center2={0.0 0.0 1.0} radius=0.25
```

Define a sphere with a center point of {0.0 0.0 0.0} and a radius of 0.25 µm, with the name sphere_1 (the sphere can be used in a subsequent etching or deposition step):

```
define_shape type=sphere name=sphere_1 center={0.0 0.0 0.0} radius=0.25
```

Define a pyramid with vertices at the points of coordinates {0.0 0.0 0.0}, {0.0 0.0 1.0}, {0.0 1.0 0.0}, {0.0 1.0 1.0}, and {0.5 0.5 1.0} (this pyramid can be used in a subsequent etching or deposition step):

```
define_shape type=cube name=pyramid point_min={0.0 0.0 0.0} \
point_max={1.0 1.0 1.0} scale_top=0
```

Define a square truncated pyramid with vertices at the points of coordinates {0.0 0.0 0.0}, {0.0 0.0 1.0}, {0.0 1.0 0.0}, {0.0 1.0 1.0}, {0.25 0.25 1.0}, {0.75 0.25 1.0}, {0.25 0.75 1.0}, and {0.75 0.75 1.0} (this pyramid can be used in a subsequent etching or deposition step):

```
define_shape type=cube name=square_truncated_pyramid \
point_min={0.0 0.0 0.0} \
point_max={1.0 1.0 1.0} scale_top=0.5
```

Define a nonsquare truncated pyramid with vertices at the points of coordinates {0.0 0.0 0.0}, {0.0 0.0 1.0}, {0.0 1.0 0.0}, {0.0 1.0 1.0}, {0.25 0.375 1.0}, {0.75 0.375 1.0}, {0.25 0.625 1.0}, and {0.75 0.625 1.0} (this pyramid can be used in a subsequent etching or deposition step):

```
define_shape type=cube name=truncated_pyramid \
point_min={0.0 0.0 0.0} point_max={1.0 1.0 1.0} \
scale_top_x=0.5 scale_top_y=0.25
```

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define_shape

Define an ellipsoid centered at the point of coordinates {0.0 0.0 0.0} and with main axes of length 0.5 μm in the x-direction, 0.2 μm in the y-direction, and 1 μm in the z-direction (this ellipsoid can be used in a subsequent etching or deposition step):

```
define_shape type=ellipsoid name=e center={0.0 0.0 0.0} \
    radius_a=0.5 radius_b=0.2 radius_c=1
```

Define a 3D elliptic hole by three axis points, $\vec{c}_1 = (0,0,2)$, $\vec{c}_2 = (0.01,0,1)$, and $\vec{c}_3 = (-0.01,0,0)$. At each height z , the xy cross-section is an ellipse, defined by two radii, a rotation, and an elliptic exponent. For example, at \vec{c}_1 , the first radius of the ellipse is 1.0, the second radius is 1.5, the rotation with respect to the x-axis is 45°, and the elliptic exponent is 2:

```
define_shape type=stacked_cylinder name=cyl \
    center_list={ 0      0      2 \
                  0.01   0      1 \
                  -0.01  0      0 } \
    radius_a_list={1.0  0.9  1.1} \
    radius_b_list={1.5  1.4  1.5} \
    rotation_list={45  50  55} \
    elliptic_exponent_list={2  2  2} \
    refinement=360
```

Define a cube rotated by Euler angles `alpha`, `beta`, and `gamma` around the z-axis, x'-axis, and z"-axis:

```
define_shape name=cube type=cube point_min={ 0.2 0.2 0.0 } \
    point_max={0.6 0.6 1.0} alpha=90 beta=-20 gamma=-100
```

Define a cube rotated by 7° around an axis specified with a point and a direction:

```
define_shape name=cube type=cube point_min={0.2 0.2 0.0} \
    point_max={0.6 0.6 1.0} axis_rotation=7 \
    direction={0.3 0.2 0.5} point={1.0 2.4 1.8}
```

Etch an asymmetric hole, given by two opposite surface lines `profile1` and `profile2`. The x-coordinates in `profile1` and `profile2` are measured with respect to a reference axis at the origin, (x,y)=(0,0), as specified by parameter `center`:

```
define_structure material=Oxide \
    point_min={ -0.4 -0.2 0.0 } \
    point_max={ 0.0 +0.2 1.0 }

define_shape name=s type=asymmetric_hole \
    profile1={ 0.00 1.0 \
               -0.10 0.9 \
               -0.18 0.8 \
               -0.20 0.7 \
               -0.20 0.5 \
               -0.19 0.4 \
               -0.20 0.2 \
               -0.25 0.1 } \
```

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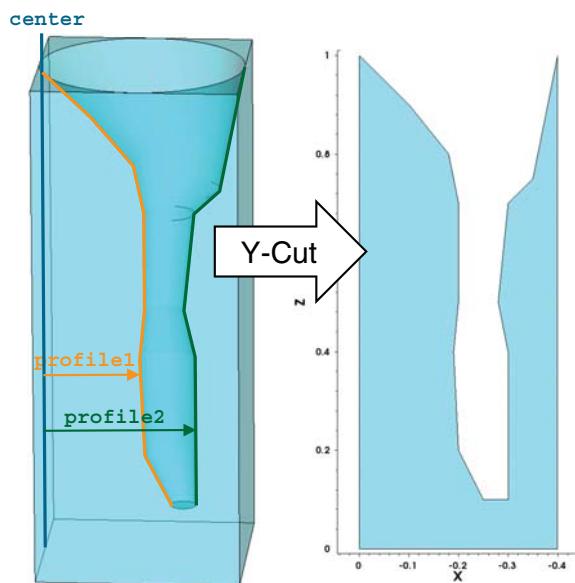
define_shape

```
profile2={-0.30 0.1 \
          -0.30 0.4 \
          -0.28 0.5 \
          -0.30 0.7 \
          -0.35 0.75 \
          -0.40 1.0} \
center={0 0} refinement=90

etch shape=s
```

[Figure 26](#) shows the resulting shape.

Figure 26 Generation of an asymmetric hole



Chapter 6: Input Commands

define_sheath_solver

define_sheath_solver

This optional command defines the numeric parameters of the solver used for a plasma sheath model. Depending on the sheath model type, different solvers are available.

Note:

Two default sheath solvers are implicitly defined and can be referenced by other commands, such as `solve_reactor` (see [solve_reactor on page 548](#)). For example:

- `default_analytic_sheath_solver` (**for** `sheath_model_type=analytic`)
- `default_circuit_sheath_solver` (**for** `sheath_model_type=circuit`)

The implicit definitions of these default solvers are equivalent to:

```
define_sheath_solver name=default_analytic_sheath_solver \
    sheath_model_type=analytic
```

```
define_sheath_solver name=default_circuit_sheath_solver \
    sheath_model_type=circuit
```

Syntax

Analytic RF sheath model (see [Analytic RF Sheath Model on page 115](#)):

```
define_sheath_solver name=<c> sheath_model_type=analytic \
    [num_angle_samples=<n>] [num_energy_samples=<n>]
```

Self-consistent circuit RF sheath model (see [Self-Consistent Circuit RF Sheath Model on page 110](#)):

```
define_sheath_solver name=<c> sheath_model_type=circuit \
    [abs_error=<n>] [discard_slow_ions=<b>] \
    [frequency_snapping_tolerance=<n>] \
    ([ied_bin_size=<n>] | [num_ied_histogram_bins=<n>]) \
    [ied_solver=<c>] \
    [initial_rf_current=<n>] [initial_sheath_width=<n>] \
    [initial_wall_potential=<n>] \
    [max_num_waveform_periods=<n>] \
    [max_rf_current_step=<n>] \
    [max_rf_voltage_step=<n>] [max_sheath_iterations=<n>] \
    [max_sheath_width_integration_steps=<n>] \
    [max_sheath_width_iterations=<n>] \
    [max_wall_potential_iterations=<n>] \
    [min_sheath_width_integration_steps=<n>] \
    [monte_carlo_random_seed=<n>] \
    [num_angle_samples=<n>] [num_energy_samples=<n>] \
    [num_inv_cdf_histogram_bins=<n>] \
    [num_monte_carlo_samples=<n>] \
    [power_relaxation_constant=<n>] [power_tolerance=<n>] \
    [rel_error=<n>] [sheath_tolerance=<n>] [time_average_solution=<b>]
```

Chapter 6: Input Commands

define_sheath_solver

Table 53 Parameters of *define_sheath_solver* command

Parameter	Description
abs_error	Sets the absolute error used for adaptive step size control during the trajectory integration in the Monte Carlo sheath solver. It applies only when <code>ied_solver=monte_carlo</code> . Type: Number Default: 10^{-6} Range: $[0, \infty[$
discard_slow_ions	Specifies whether to discard trajectories, which intersect the oscillating RF sheath boundary, in the Monte Carlo sheath solver. Type: Boolean Default: <code>true</code>
frequency_snapping_tolerance	When using time-dependent waveforms (from a bulk simulation with pulsed power) as input to the sheath model, this parameter sets the tolerance used when trying to find the least common multiple period between the input waveforms (densities and electron temperature) and the bias waveforms (bias current, voltage, or power). Type: Number Default: 0.01 Range: $[0, \infty[$
ied_bin_size	Sets the energy resolution of the ion energy distribution (IED) histogram. You can specify either <code>ied_bin_size</code> or <code>num_ied_histogram_bins</code> . Type: Number Default: none Range: $[0, \infty[$
ied_solver	Sets the method used to compute the IED of the ions crossing the sheath layer. Options are <code>analytic</code> and <code>monte_carlo</code> . This parameter is available only for <code>sheath_model_type=circuit</code> . Type: Character Default: <code>monte_carlo</code>

Chapter 6: Input Commands

define_sheath_solver

Table 53 Parameters of define_sheath_solver command (Continued)

Parameter	Description
initial_rf_current	Sets the initial guess of the RF current. Type: Number Default: 3 Range:]0,∞[Unit: A
initial_sheath_width	Sets the initial guess of the sheath width. Type: Number Default: 10^{-4} Range:]0,∞[Unit: m
initial_wall_potential	Sets the initial guess of the sheath wall potential. Type: Number Default: -10 Range:]0,∞[Unit: V
max_num_waveform_periods	When using time-dependent density and electron temperature waveforms from a bulk simulation with pulsed power as input to the sheath model, this parameter sets the maximum number of periods considered when trying to find the least common multiple period between the input waveforms (densities and electron temperature) and the bias waveforms (bias current, voltage, or power). Type: Number Default: 100 Range: [1, ∞)
max_rf_current_step	If you specify rf_bias_power with bias_mode=current_driven, then you can set the maximum-allowed relative change of the RF bias current during convergence toward the specified RF bias power by using this parameter. Type: Number Default: 0.05 Range:]0, ∞)

Chapter 6: Input Commands

define_sheath_solver

Table 53 Parameters of *define_sheath_solver* command (Continued)

Parameter	Description
max_rf_voltage_step	If you specify <code>rf_bias_power</code> with <code>bias_mode=voltage_driven</code> , then you can set the maximum-allowed relative change of the RF bias voltage during convergence toward the specified RF bias power by using this parameter. Type: Number Default: 0.05 Range:]0, ∞)
max_sheath_iterations	Sets the maximum number of iterations to obtain a self-consistent overall sheath solution. Type: Number Default: 10^7 Range: [1, ∞ [
max_sheath_width_integration_steps	Sets the maximum number of integration steps to solve for the sheath width. Type: Number Default: 500 Range: [1, ∞ [
max_sheath_width_iterations	Sets the maximum number of iterations to solve for the sheath width. Type: Number Default: 8 Range: [1, ∞]
max_wall_potential_iterations	Sets the maximum number of iterations to solve for the wall potential. Type: Number Default: 8 Range: [1, ∞]
min_sheath_width_integration_steps	Sets the minimum number of integration steps to solve for the sheath width. Type: Number Default: 50 Range: [1, ∞ [

Chapter 6: Input Commands

define_sheath_solver

Table 53 Parameters of define_sheath_solver command (Continued)

Parameter	Description
monte_carlo_random_seed	Sets the random seed used to sample the IED by the Monte Carlo sheath solver. This parameter applies only when ied_solver=monte_carlo. Type: Number Default: 42 Range: [0, ∞)
name	Sets the name of the solver. This name is used to reference the solver in other commands, such as solve_reactor (see solve_reactor on page 548). Type: Character Default: none
num_angle_samples	Sets the number of angle samples used to resolve the energy-angular distribution. Type: Number Default: 180 Range: [2, ∞[
num_energy_samples	Sets the number of energy samples used to resolve the energy-angular distribution. Type: Number Default: 1000 Range: [2, ∞[
num_ied_histogram_bins	Sets the number of bins in the IED histogram. You can specify either ied_bin_size or num_ied_histogram_bins. Type: Number Default: 1000 Range: [2, ∞[
num_inv_cdf_histogram_bins	Sets the number of bins of the inverse cumulative distribution function (CDF) histogram corresponding to the IED. Type: Number Default: 1000 Range: [1, ∞]

Chapter 6: Input Commands

define_sheath_solver

Table 53 Parameters of define_sheath_solver command (Continued)

Parameter	Description
num_monte_carlo_samples	Sets the number of samples used to sample the ion energy distribution in the Monte Carlo sheath solver. You can specify this parameter only if ied_solver=monte_carlo. Type: Number Default: 10000 Range: [2, ∞)
power_relaxation_constant	If you specify rf_bias_power, then you can use this parameter to set the characteristic scale of the relaxation toward the specified RF bias power. Type: Number Default: 100 Range:]0, ∞)
power_tolerance	Sets the tolerance for the convergence criterion of the RF bias power. Type: Number Default: 10^{-3} Range:]0, ∞ [
rel_error	Sets the relative error used for adaptive step size control during the trajectory integration in the Monte Carlo sheath solver. You can specify this parameter only if ied_solver=monte_carlo. Type: Number Default: 10^{-6} Range:]0, ∞ [
sheath_model_type	Sets the type of the sheath model to solve. Options are: <ul style="list-style-type: none">• analytic• circuit Type: Character Default: none
sheath_tolerance	Sets the tolerance for the convergence criterion of the sheath potential. Type: Number Default: 10^{-3} Range:]0, ∞ [

Chapter 6: Input Commands

define_sheath_solver

Table 53 Parameters of *define_sheath_solver* command (Continued)

Parameter	Description
time_average_solution	When using time-dependent density and electron temperature waveforms from a bulk simulation with pulsed power as input to the sheath model, this parameter specifies whether the sheath solution, consisting of time-dependent periodic waveforms, should be averaged in time. Type: Boolean Default: true

Examples

```
define_sheath_solver name=s2 sheath_model_type=analytic \
    num_angle_samples=180 num_energy_samples=1000

define_sheath_solver name=s1 sheath_model_type=circuit \
    initial_sheath_width=1e-4<m> initial_wall_potential=-10<V> \
    initial_rf_current=3<A> max_sheath_iterations=1000 \
    max_sheath_width_iterations=8 \
    min_sheath_width_integration_steps=10 \
    max_sheath_width_integration_steps=100 \
    max_wall_potential_iterations=8 \
    num_angle_samples=180 \
    num_energy_samples=1000 num_ied_histogram_bins=200 \
    num_inv_cdf_histogram_bins=100 sheath_tolerance=1e-3 \
    power_tolerance=1e-2
```

Chapter 6: Input Commands

define_species_distribution

define_species_distribution

This command defines a new energy and angular distribution (EAD) that can be used in a reaction model. As a special case, it allows you to define angular distributions that are energy independent.

Syntax: Analytic and Tabular EADs

In the following syntax examples, a distribution is energy dependent only if you explicitly specify energy-related parameters:

```
<energy_parameters>=
  energy_center=<n> energy_center_weight=<n> energy_max=<c>
  energy_min=<c> energy_max_weight=<n> energy_min_weight=<n>
```

Otherwise, the distribution is assumed to be energy independent.

You can specify the following types of energy distribution:

- Monoenergetic: If you set the same value for `energy_min` and `energy_max`, then all particles will have the same energy.
- Uniform: You can define a uniform energy window by setting `energy_min` and `energy_max`.
- Bimodal: You can define a bimodal energy distribution by specifying the three characteristic points: the two peaks at `energy_min` and `energy_max`, and the minimum position at `energy_center`.

To specify the relative heights between the peaks and the minimum, use `energy_min_weight`, `energy_max_weight`, and `energy_center_weight`. (The weights do not define the absolute values of the final energy- and angle-dependent flux distribution (IEAD) used by the PMC method. This is because the actual amplitude of the IEAD is determined by the parameter flux, which is defined as the integral of the IEAD over all energies and angles.)

Define a distribution whose angular-dependent part is described by [Equation 5 on page 49](#):

```
define_species_distribution exponent=<c> flux=<c> name=<c> \
  species=<c> [<energy_parameters>] [orientation=<v>] \
  [sampling_time_step=<n>]
```

As an alternative to the exponent parameter, you can specify the characteristic width of the angular distribution in [Equation 5](#) by using the `angle_spread` parameter. This parameter is defined such that 68.3% of the particles have an angle smaller than `angle_spread` (in analogy to the first confidence interval of a Gaussian distribution):

```
define_species_distribution angle_spread=<n> flux=<c> name=<c> \
  species=<c> [<energy_parameters>] [orientation=<v>] \
  [sampling_time_step=<n>]
```

Chapter 6: Input Commands

define_species_distribution

Define a distribution that specifies particles traveling along the vertical direction:

```
define_species_distribution flux=<c> name=<c> species=<c> \
    unidirectional=<b> \
    [<energy_parameters>] [orientation=<v>] [sampling_time_step=<n>]
```

Define a distribution whose angular-dependent part is described by tabular data:

```
define_species_distribution flux=<c> name=<c> species=<c> table=<v> \
    [angle_unit=<c>] [<energy_parameters>] \
    [orientation=<v>] [sampling_time_step=<n>]
```

You can define an azimuth-dependent angular distribution with an anisotropic exponent. The analytic expression for anisotropic exponents is given by:

$$f(\theta, \phi) = A \cos^{m(\phi)}(\theta) \quad (87)$$

where the exponent depends on the azimuth ϕ as given by

$$m(\phi) = m_x \cos^2(\phi) + m_y \sin^2(\phi).$$

Therefore, the exponent takes the value m_x in the x-direction and m_y in the y-direction. An additional azimuthal rotation $\phi \rightarrow \phi - \phi_0$ allows you to orientate x- and y-anisotropy axes along an arbitrary direction (see [Figure 28 on page 351](#)).

Define an azimuth-dependent species distribution:

```
define_species_distribution type=azimuthal exponent_x=<c> \
    exponent_y=<c> flux=<c> name=<c> species=<c> \
    [<energy_parameters>] [orientation=<v>] [rotation=<n>]
```

Syntax: EADs From Plasma Models

An energy and angular distribution can also be computed by the Benoit-Cattin plasma sheath model for capacitively coupled plasma (CCP) reactors [\[9\]](#)[\[10\]](#)[\[11\]](#). This model depends on the parameters of the plasma reactor, such as the temperature T_e of the electrons, the ion bulk density n_i , mass m_i , and temperature T_i of the plasma ions, and the applied RF voltage $V(t) = V_{rf} \sin(2\pi f_{rf}t)$, where V_{rf} denotes the amplitude of the RF voltage and f_{rf} is the RF pulsing frequency. The distribution can be defined with the following command:

```
define_species_distribution type=ccp_sheath \
    electron_temperature=<n> \
    ion_bulk_density=<n> ion_mass=<n> ion_temperature=<n> name=<c> \
    rf_frequency=<n> rf_voltage=<n> species=<c> \
    [flux=<c>] [sampling_time_step=<n>]
```

As an alternative to the applied RF voltage V_{rf} , you can specify the sheath voltage $V_{rf}(t) = V_{DC} + V_{AC} \sin(2\pi f_{ft}t)$ by defining the AC sheath voltage V_{AC} and the DC sheath voltage V_{DC} :

```
define_species_distribution type=ccp_sheath ac_voltage=<n> \
    dc_voltage=<n> electron_temperature=<n> \
```

Chapter 6: Input Commands

define_species_distribution

```
ion_bulk_density=<n> ion_mass=<n> \
ion_temperature=<n> name=<c> rf_frequency=<n> species=<c> \
[flux=<c>] [sampling_time_step=<n>]
```

See [Analytic RF Sheath Model on page 115](#).

For inductively coupled plasma (ICP) reactors, the energy and angular distribution is computed by the Edelberg–Aydil plasma sheath model [10][12]. This model also depends on reactor parameters such as the electrode area A , the electron temperature T_e , the ion bulk density n_i , mass m_i , and temperature T_i of the plasma ions, and the applied RF current $I(t) = I_{rf} \sin(2\pi f_{rf} t)$, where I_{rf} denotes the amplitude of the RF current and f_{rf} is the RF pulsing frequency.

The distribution can be defined with the following command:

```
define_species_distribution type=icp_sheath electrode_area=<n> \
electron_temperature=<n> ion_bulk_density=<n> ion_mass=<n> \
ion_temperature=<n> name=<c> rf_current=<n> rf_frequency=<n> \
species=<c> \
[flux=<c>] [sampling_time_step=<n>]
```

Instead of specifying the applied RF current I_{rf} , you can specify the RF bias power P_{rf} :

```
define_species_distribution type=icp_sheath electrode_area=<n> \
electron_temperature=<n> ion_bulk_density=<n> ion_mass=<n> \
ion_temperature=<n> name=<c> rf_frequency=<n> rf_power=<n> \
species=<c> \
[flux=<c>] [sampling_time_step=<n>]
```

See [Self-Consistent Circuit RF Sheath Model on page 110](#).

Define a species distribution from the solution of a plasma model (see [Chapter 4 on page 99](#) and [solve_reactor on page 548](#)):

```
define_species_distribution type=plasma name=<c> \
(solution=<c> | solution_file=<c>) species=<c> [flux=<c>]
```

Syntax: EADs From Files

Import an energy and angular distribution computed by the Plasma Chemistry Monte Carlo (PCMC) module of the HPEM plasma simulator [13][14]:

```
define_species_distribution hpem_file=<c> name=<c> species=<c> \
[energy_max=<c> energy_min=<c> flux=<c> hpem_material_index=<n> \
hpem_species=<c>] [sampling_time_step=<n>]
```

Define an energy-independent angular distribution by integrating an energy and angular distribution computed by HPEM:

```
define_species_distribution hpem_file=<c> \
integration_energy_max=<n> \
integration_energy_min=<n> name=<c> species=<c> \
```

Chapter 6: Input Commands

define_species_distribution

```
[flux=<c> hpem_material_index=<n> hpem_species=<c>] \
[sampling_time_step=<n>]
```

Import an energy and angular distribution from an EAD file (see [Appendix B on page 616](#)):

```
define_species_distribution type=ead_file file=<c> name=<c> \
species=<c> \
[energy_min=<c> energy_max=<c>] [flux=<c>] \
[sampling_method=<c>] [sampling_time_step=<n>]
```

Syntax: Combining Distributions

Previously defined species distributions can be combined into a single species distribution by summing the flux distributions of individual distributions with the following command:

```
define_species_distribution type=sum distributions=<l> name=<c> \
species=<c> [flux=<c>]
```

Table 54 Parameters of define_species_distribution command

Parameter	Description
ac_voltage	Sets the AC sheath voltage. This parameter applies only if type=ccp_sheath and if rf_voltage is not specified. Type: Number Default: none Range:]0, ∞[Unit: V
angle_spread	Sets the characteristic width of the angular distribution $\cos^m(\theta)$. The angle spread is defined such that 68.3% of the particles have an angle smaller than angle_spread. Type: Number Default: none Range:]0, 55.716] Unit: degree
angle_unit	Sets the unit of the angles listed in the table parameter. Options are: <ul style="list-style-type: none">• deg• rad Type: Character Default: deg

Chapter 6: Input Commands

define_species_distribution

Table 54 Parameters of define_species_distribution command (Continued)

Parameter	Description
dc_voltage	Sets the DC sheath voltage. This parameter applies only if type=ccp_sheath and if rf_voltage is not specified. Type: Number Default: none Range:]0, ∞[Unit: V
distributions	Specifies a list of lists, containing the names and species of the flux distributions to be summed. Format: {{distribution1 species1} {distribution2 species2} ... } This parameter applies only if type=sum. Type: List Default: none
electrode_area	Sets the area of the electrode. This parameter applies only if type=icp_sheath. Type: Number Default: none Range:]0, ∞[Unit: cm ²
electron_temperature	Sets the electron temperature at the plasma sheath edge. This parameter applies if either type=ccp_sheath or type=icp_sheath. Type: Number Default: none Range:]0, ∞[Unit: eV
energy_center	Sets the position of the energy minimum when defining a bimodal energy distribution. Type: Number Default: none Range:]0, ∞[Unit: eV

Chapter 6: Input Commands

define_species_distribution

Table 54 Parameters of *define_species_distribution* command (Continued)

Parameter	Description
energy_center_weight	<p>Sets the height of a bimodal energy distribution at the energy specified by <code>energy_center</code>. This parameter can be specified only if <code>energy_center</code> is specified.</p> <p>Type: Number</p> <p>Default: 1</p> <p>Range: $[0, \infty[$</p>
energy_max	<p>Sets the maximum energy of the energy distribution. When <code>hpem_file</code> is specified, <code>energy_max</code> sets the maximum energy to take into account when reading the specified HPEM output file.</p> <p>When <code>type=ead_file</code>, <code>energy_max</code> sets the upper energy limit of the EAD. Energy values above this limit are not considered during import.</p> <p>Type: Character</p> <p>Default: ∞ when <code>type=ead_file</code> or <code>hpem_file</code> is used; otherwise, none</p> <p>Range: Time-dependent expression, evaluating to $[0, \infty[$ and not smaller than the value of the time-dependent expression <code>energy_min</code> at the same time</p> <p>Unit: eV</p>
energy_max_weight	<p>Sets the height of a bimodal energy distribution at the energy specified by <code>energy_max</code>. This parameter can be specified only if <code>energy_max</code> is specified.</p> <p>Type: Number</p> <p>Default: 1</p> <p>Range: $[0, \infty[$</p>

Chapter 6: Input Commands

define_species_distribution

Table 54 Parameters of define_species_distribution command (Continued)

Parameter	Description
energy_min	<p>Sets the minimum energy of the energy distribution.</p> <p>When <code>hpem_file</code> is specified, <code>energy_min</code> sets the minimum energy to take into account when reading the specified HPEM output file.</p> <p>When <code>type=ead_file</code>, <code>energy_min</code> sets the lower energy limit of the EAD. Energy values below this limit are not considered during import.</p> <p>Type: Character</p> <p>Default: 0 when <code>type=ead_file</code> or <code>hpem_file</code> is used; otherwise, none</p> <p>Range: Time-dependent expression, evaluating to $[0, \infty[$ and not larger than the value of the time-dependent expression <code>energy_max</code> at the same time</p> <p>Unit: eV</p>
energy_min_weight	<p>Sets the height of a bimodal energy distribution at the energy specified by <code>energy_min</code>.</p> <p>This parameter can be specified only if <code>energy_min</code> is specified.</p> <p>Type: Number</p> <p>Default: 1</p> <p>Range: $[0, \infty[$</p>
exponent	<p>Sets the expression of the exponent of the angular distribution ($\cos^m(\theta)$) of the species.</p> <p>Type: Character</p> <p>Default: none</p> <p>Range: Time-dependent expression, evaluating to $[1, \infty[$</p>
exponent_x	<p>Sets the exponent in the x-direction.</p> <p>Note: This parameter applies only if <code>type=azimuthal</code>.</p> <p>Type: Character</p> <p>Default: none</p> <p>Range: Time-dependent expression, evaluating to $[1, \infty[$</p>

Chapter 6: Input Commands

define_species_distribution

Table 54 Parameters of define_species_distribution command (Continued)

Parameter	Description
exponent_y	<p>Sets the exponent in the y-direction.</p> <p>Note: This parameter applies only if type=azimuthal.</p> <p>Type: Character Default: none Range: Time-dependent expression, evaluating to [1, ∞[</p>
file	<p>Sets the path to the EAD file to be imported.</p> <p>Note: This parameter applies only if type=ead_file.</p> <p>Type: Character Default: none</p>
flux	<p>Sets the expression of the number of molecules or atoms of the specified species entering the top face of the simulation domain per unit time and area. This parameter operates as follows:</p> <ul style="list-style-type: none"> • If specified when reading data from an HPEM file, flux overwrites the flux specified by the HPEM file. • If specified when defining the sum of previously defined distributions, flux overwrites the total flux. • If specified when using the Benoit-Cattin or Edelberg–Aydil plasma sheath model, flux overwrites the flux computed from the plasma sheath model. • If specified when importing an energy and angular distribution from an EAD file, flux overwrites the flux specified in the EAD file. • If specified when defining the distribution from a plasma model, flux overwrites the flux computed by the plasma model. <p>Type: Character Default: none Range: Time-dependent expression, evaluating to [0, ∞[Unit: mol/s/m²</p>
hpeM_file	<p>Sets the name of the file containing the output of the PCMC module of the HPEM simulator, that is, the energy and angular distributions.</p> <p>Type: Character Default: none</p>

Chapter 6: Input Commands

define_species_distribution

Table 54 Parameters of *define_species_distribution* command (Continued)

Parameter	Description
hpem_material_index	Sets the index of the HPEM material where the HPEM index species was measured. Type: Number Default: none
hpem_species	Sets the name of the HPEM species that the angular distributions must read. If omitted, the HPEM species with the name provided by the <i>species</i> parameter will be used. Type: Character Default: none
integration_energy_max	Sets the maximum energy to take into account when integrating an energy and angular distribution. Type: Number Default: none Range: [0, ∞[Unit: eV
integration_energy_min	Sets the minimum energy to take into account when integrating an energy and angular distribution. Type: Number Default: none Range: [0, ∞[Unit: eV
ion_bulk_density	Sets the number of ions per volume in the plasma bulk. This parameter applies only if <i>type=ccp_sheath</i> or <i>type=icp_sheath</i> . Type: Number Default: none Range:]0, ∞[Unit: 1/cm ³
ion_mass	Sets the mass of the ion species in the plasma. This parameter can be used for either <i>type=ccp_sheath</i> or <i>type=icp_sheath</i> . Type: Number Default: none Range:]0, ∞[Unit: g

Chapter 6: Input Commands

define_species_distribution

Table 54 Parameters of define_species_distribution command (Continued)

Parameter	Description
ion_temperature	Sets the ion temperature at the sheath edge. This parameter applies only if <code>type=ccp_sheath</code> or <code>type=icp_sheath</code> . Type: Number Default: none Range:]0, ∞[Unit: eV
name	Sets the name of the energy and angular distribution. Type: Character Default: none
orientation	Sets the orientation of the center point of the source distribution. The orientation is specified by a pair of angles (θ, ϕ), where: <ul style="list-style-type: none"> • $\theta \in [0, 90]$ denotes the polar angle ($\theta = 0$ corresponds to the negative z-axis). • $\phi \in [-180, 180]$ denotes the azimuth angle ($\phi = 0$ corresponds to the x-axis of the simulation coordinate system). See Figure 27 on page 350 . Type: Vector Default: (0, 0) Range: Time-dependent expression, evaluating to [0, 90] × [-180, 180] Unit: degree
rf_current	Sets the amplitude of the sinusoidal current applied at the discharge. This parameter can be used only for <code>type=icp_sheath</code> and if <code>rf_power</code> is not specified. Type: Number Default: none Range:]0, ∞[Unit: A
rf_frequency	Sets the applied radio frequency of the plasma source. This parameter applies only if <code>type=ccp_sheath</code> or <code>type=icp_sheath</code> . Type: Number Default: none Range:]0, ∞[Unit: Hz

Chapter 6: Input Commands

define_species_distribution

Table 54 Parameters of define_species_distribution command (Continued)

Parameter	Description
rf_power	Sets the amplitude of the sinusoidal current applied at the discharge. This parameter applies only if type=icp_sheath and if rf_current is not specified. Type: Number Default: none Range:]0, ∞[Unit: W
rf_voltage	Sets the total voltage across the discharge. Alternatively, use ac_voltage and dc_voltage to specify the sheath voltage. This parameter applies only if type=ccp_sheath. Type: Number Default: none Range:]0, ∞[Unit: V
rotation	Sets an azimuthal rotation of the elliptical distribution with respect to the simulation coordinate system. A rotation of 0° corresponds to an ellipse with exponent_x aligned in the x-direction and exponent_y aligned in the y-direction. Type: Number Default: 0 Range: Time-dependent expression, evaluating to [-180, 180] Unit: degree
sampling_method	Sets the method used to sample the species distribution. Options are: <ul style="list-style-type: none">• inverse_cdf• rejection This parameter applies only if type=ead_file. Type: Character Default: inverse_cdf

Chapter 6: Input Commands

define_species_distribution

Table 54 Parameters of define_species_distribution command (Continued)

Parameter	Description
sampling_time_step	<p>Sets the smallest time step used to sample the time-dependent expressions of energy_max, energy_min, exponent, exponent_x, exponent_y, flux, orientation, and rotation.</p> <p>Note:</p> <p>This parameter is mandatory when any of the values of the energy_max, energy_min, exponent, exponent_x, exponent_y, flux, orientation, or rotation parameters is a time-dependent expression.</p> <p>An expression is considered time dependent if it contains the t string (see Syntax for Expressions on page 354). Otherwise, it is time independent.</p> <p>Type: Number Default: none Unit: minute</p>
solution	<p>Sets the name of the solution of the plasma model, specified in the solve_reactor command. It can be specified only if type=plasma. You can specify either solution or solution_file.</p> <p>Type: Character Default: none</p>
solution_file	<p>Sets the name of the file containing the solution of the plasma model.</p> <p>It can be specified only if type=plasma.</p> <p>You can specify either solution or solution_file.</p> <p>Type: Character Default: none</p>
species	<p>Sets the name of the species for which the distribution is defined. If the distribution is to be defined from the solution of a plasma model (type=plasma), the name must already exist as defined in the add_species command of the plasma model.</p> <p>Type: Character Default: none</p>
table	<p>Sets the tabular format of the distribution. The same format must be used as for the table parameter of the define_iad command (see define_iad on page 274).</p> <p>Type: Vector Default: none</p>

Chapter 6: Input Commands

define_species_distribution

Table 54 Parameters of define_species_distribution command (Continued)

Parameter	Description
type	<p>Options are:</p> <ul style="list-style-type: none">azimuthal: Defines an azimuth-dependent distribution. See Figure 28 on page 351.ccp_sheath: Specifies the use of the Benoit-Cattin plasma sheath model for defining the species distribution.ead_file: Specifies the import of an EAD file.icp_sheath: Specifies the use of the Edelberg–Aydil plasma sheath model for defining the species distribution.plasma: Specifies that the distribution comes from the solution of a plasma model.sum: Specifies that the listed species distributions are combined into a single species distribution. <p>Type: Character Default: none</p>
unidirectional	<p>Specifies whether all the molecules or atoms are distributed along the vertical direction.</p> <p>Type: Boolean Default: false</p>

Description

To ease the reuse of measured or simulated data, the definition of species distributions is not part of any model. Species distributions are bound to reaction models when a machine using a reaction model is defined (see [define_etch_machine on page 242](#)).

Examples: Analytic EADs

For example, the following command specifies that atoms of species Ar travel in the reactor along the vertical direction and are energy independent. The flux of Ar atoms entering the reactor is set to 10^{-4} mol/s/m²:

```
define_species_distribution flux=1e-4 name=my_dist species=Ar \
    unidirectional=true
```

An energy-independent angular distribution according to [Equation 5 on page 49](#) with $m = 1000$ can be set to species Ar with the following command:

```
define_species_distribution exponent=1000 flux=1e-4 name=my_dist \
    species=Ar
```

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define_species_distribution

To specify an energy and angular distribution describing molecules of species F2 moving isotropically in the reactor and with energy uniformly distributed between 10 eV and 20 eV, use the command:

```
define_species_distribution exponent=1 flux=1e-4 name=my_dist \
    species=F2 energy_min=10 energy_max=20
```

Figure 27 illustrates the definition of `orientation={theta phi}`, where `theta` defines the polar angle, and `phi` defines the azimuth angle of the central axis of the ion angle distribution; `theta=0` corresponds to the z-axis and `phi=0` corresponds to the x-axis of the simulation coordinate system.

To specify an energy and angular distribution describing molecules of species Ar+ with a polar angle spread of 10° and a bimodal energy distribution (with peaks at 10 eV and 100 eV with heights 10 and 20, and with a minimum at 50 eV with height 1), use:

```
define_species_distribution angle_spread=10 flux=1e-4 \
    name=my_dist species=Ar+ \
    energy_min=10 energy_max=100 \
    energy_min_weight=10 energy_max_weight=20 \
    energy_center=50 energy_center_weight=1
```

Note:

The energy weights are not absolute flux values, since the distribution is normalized to the total flux, given by the parameter `flux`.

Figure 27 *Definition of orientation={theta phi}*

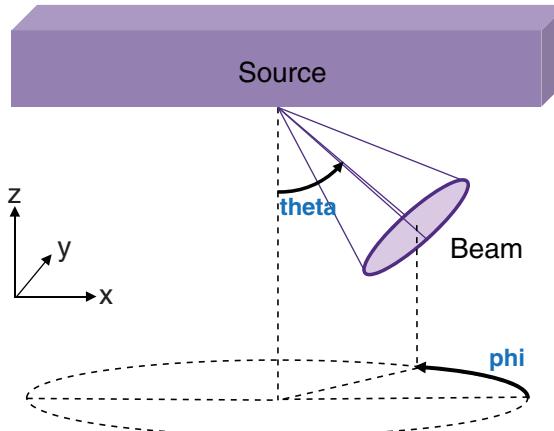
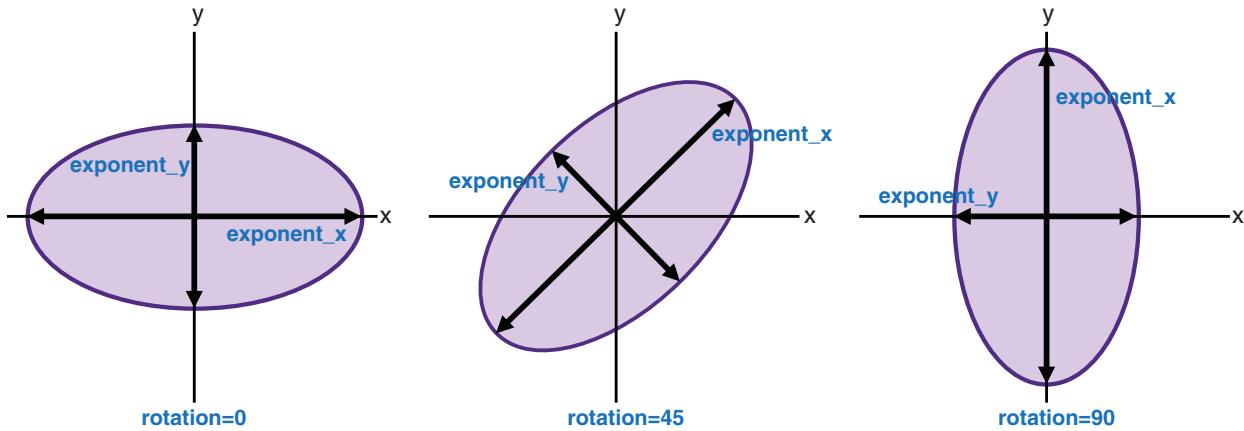


Figure 28 illustrates the definition of `type=azimuthal`, the azimuth-dependent species distribution.

Chapter 6: Input Commands

define_species_distribution

Figure 28 Definition of type=azimuthal



The flux distribution is shown at a fixed height z (top view), such that the isolines of the distribution take the shape of an ellipse. The `exponent_x` and `exponent_y` parameters define the exponents of the angle distribution along the two principal axes of the ellipse, respectively. The optional parameter `rotation` can be used to change the azimuthal orientation of the ellipse in the xy plane. If `rotation=0`, `exponent_x` corresponds to the x -axis and `exponent_y` corresponds to the y -axis of the simulation coordinate system.

Examples: HPEM Simulator

An energy and angular distribution computed by the PCMC module of the HPEM simulator for species AR^+ and stored in a file named `pcmc.prof` can be imported with the following command:

```
define_species_distribution name=my_dist species=AR^ \
    hpeM_file=pcmc.prof
```

Since the `flux` parameter is not specified, the flux of species AR^+ used in the simulation of a reaction model will be determined from the specified HPEM output.

When the `flux` parameter is specified, its value is used as the flux of the species distribution read from the HPEM output. For example, the following command defines an energy and angular distribution for species AR^+ as computed by the HPEM simulator, but with the flux equal to 10^{-3} mol/s/m²:

```
define_species_distribution name=my_dist species=AR^ flux=1e-3 \
    hpeM_file=pcmc.prof
```

When parameters `energy_min` and `energy_max` are not specified, all the energy levels available in the HPEM output are imported. You can limit the imported energy levels to those included in the range specified by parameters `energy_min` and `energy_max`.

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define_species_distribution

For example, the following command imports only the energy levels between 100 eV and 120 eV:

```
define_species_distribution name=my_dist species=AR^ \
    hpem_file=pcmc.prof energy_min=100 energy_max=120
```

Data computed by the HPEM simulator for one species can be used to define the distributions of multiple reaction model species. For example, the following commands define the energy and angular distributions of the reaction model species AR_high_energy and AR_low_energy using data computed by the HPEM simulator for the HPEM species named AR^:

```
define_species_distribution name=my_dist species=AR_high_energy \
    hpem_species=AR^ hpem_file=pcmc.prof energy_min=150 energy_max=200
```

```
define_species_distribution name=my_dist species=AR_low_energy \
    hpem_species=AR^ hpem_file=pcmc.prof energy_min=50 energy_max=100
```

You can also define an energy-independent angular distribution from an energy- and angular-dependent distribution computed by the HPEM simulator. For example:

```
define_species_distribution name=my_dist species=AR^ \
    hpem_file=pcmc.prof integration_energy_min=150 \
    integration_energy_max=200
```

This command defines an energy-independent angular distribution for species AR^ obtained as the integral over the energy of the data specified for this species in the pcmc.prof file. The parameters integration_energy_min and integration_energy_max specify the integration range.

Examples: Benoit-Cattin Plasma Sheath Model

An energy and angular distribution computed by the Benoit-Cattin model for species Ar with ion mass $m_i = 6.63 \cdot 10^{-23}$ g, ion temperature $T_i = 0.33$ eV, and ion bulk density $n_i = 2.8 \cdot 10^9$ cm $^{-3}$, moving in a CCP discharge with electron temperature $T_e = 3.3$ eV, applied RF voltage $V_{rf} = 500$ V, and $f_{rf} = 80$ MHz can be specified with the following command:

```
define_species_distribution name=my_dist species=Ar type=ccp_sheath \
    electron_temperature=3.3 ion_bulk_density=2.8e9 ion_mass=6.63e-23 \
    ion_temperature=0.33 rf_frequency=80e6 rf_voltage=500
```

Instead of specifying the applied RF voltage V_{rf} , you can define the sheath voltage $V_{rf}(t) = V_{DC} + V_{AC} \sin(2\pi f_{rf} t)$ by defining the AC sheath voltage V_{AC} and the DC sheath voltage V_{DC} . For example, for $V_{AC} = 415$ V and $V_{DC} = 207.5$ V, specify the following command:

```
define_species_distribution name=my_dist species=Ar type=ccp_sheath \
    ac_voltage=415 dc_voltage=207.5 electron_temperature=3.3 \
    ion_bulk_density=2.8e9 ion_mass=6.63e-23 ion_temperature=0.33 \
    rf_frequency=80e6
```

Chapter 6: Input Commands

```
define_species_distribution
```

Examples: Edelberg–Aydil Plasma Sheath Model

An energy and angular distribution computed by the Edelberg–Aydil model for species Ar with ion mass $m_i = 6.63 \cdot 10^{-23}$ g, ion temperature $T_i = 0.33$ eV, and ion bulk density $n_i = 2.8 \cdot 10^9 \text{ cm}^{-3}$, moving in an ICP discharge with electrode area $A = 325 \text{ cm}^2$, electron temperature $T_e = 3.3$ eV, applied RF current $I_{rf} = 6.175$ A, and $f_{rf} = 80$ MHz can be specified with the following command:

```
define_species_distribution name=my_dist species=Ar type=icp_sheath \
    electrode_area=325 electron_temperature=3.3 \
    ion_bulk_density=2.8e9 ion_mass=6.63e-23 ion_temperature=0.33 \
    rf_current=6.175 rf_frequency=80e6
```

Instead of specifying the applied RF current I_{rf} , you can define the applied RF bias power P_{rf} . For example, for $P_{rf} = 80$ W, specify the following command:

```
define_species_distribution name=my_dist species=Ar type=icp_sheath \
    electrode_area=325 electron_temperature=3.3 \
    ion_bulk_density=2.8e9 ion_mass=6.63e-23 ion_temperature=0.33 \
    rf_frequency=80e6 rf_power=80
```

Examples: Importing an EAD File

To import a distribution function from an EAD file `my_sd.txt`, use the following command:

```
define_species_distribution type=ead_file name=sd species=Ar \
    file=my_sd.txt
```

Examples: Combining Species Distributions

To combine species distributions into a single species distribution:

```
define_species_distribution name=sd1 species=CF2 exponent=1 flux=0.001
define_species_distribution name=sd2 species=CF3 exponent=5 flux=0.05
define_species_distribution name=sd_sum species=CFx type=sum \
    distributions= {{sd1 CF2} {sd2 CF3}}
define_species_distribution name=sd_sum2 species=CFx type=sum \
    distributions= {{sd1 CF2} {sd2 CF3}} flux=1e-3
```

Examples: Plasma Model Distributions

```
define_species_distribution name=sd species=Ar+ type=plasma \
    solution=sol1
define_species_distribution name=sd species=Ar+ type=plasma \
    solution=sol1 flux=1e-3
```

Chapter 6: Input Commands

define_species_distribution

Syntax for Expressions

For details about time-dependent expressions, see [Syntax for Expressions on page 139](#).

In addition, you can specify the unit of the numeric value to which an expression evaluates. If `expr` denotes an expression, then this can be accomplished using the following syntax:

`(expr)<expression_unit>`

If `expr` is a number, then you can omit the parentheses enclosing it. The possible values for `<expression_unit>` depend on the parameter to which the expression is assigned:

- When assigned to the `flux` parameter, `<expression_unit>` can be one of the following:
 - mol/m²/s (default)
 - mol/cm²/s
 - mol/m²/min
 - mol/cm²/min
- When assigned to the `energy_max` or `energy_min` parameter, `<expression_unit>` can be either eV (default) or J.

Examples

The following command defines a square pulse-shaped time-dependent flux with a period of 1 minute and a duty cycle of 0.8 for a distribution whose angular-dependent part is described by [Equation 5 on page 49](#). The smallest time step used to sample the defined time-dependent flux is set to 0.1 minutes:

```
define_species_distribution name=sd species=Ar exponent=1 \
    flux="square_pulse(t, 1e-3, 0.0, 1.0, 0.8)" sampling_time_step=0.1
```

The following command defines a square pulse-shaped time-dependent flux with a period of 1 s and a duty cycle of 0.8 for a distribution whose angular-dependent part is described by [Equation 5](#). The smallest time step used to sample the defined time-dependent flux is set to 0.1 minutes:

```
define_species_distribution name=sd species=Ar exponent=1 \
    flux="square_pulse(t<s>, 1e-3, 0.0, 1.0, 0.8)" \
    sampling_time_step=0.1
```

The following command defines a species distribution whose angular-dependent part is described by [Equation 5 on page 49](#), with:

- A flux of 1 mole per cm² per second
- A square pulse-shaped time-dependent exponent

Chapter 6: Input Commands

define_species_properties

- A uniform energy distribution between 10 eV and a time-dependent upper energy limit expressed in joules
- The smallest time step used to sample all time-dependent parameters of the distribution is set to 0.1 minutes

```
define_species_distribution name=sd species=Ar \
    exponent="square_pulse(t, 1000, 1, 2.0, 0.75)" \
    flux=1<mol/cm2/s> energy_min=10 \
    energy_max="(2e-19*square_pulse(t,50,30,1.0,0.5))<J>" \
    sampling_time_step=0.1
```

define_species_properties

This command defines the properties of a species used in a reaction model.

When not simulating charge-up, it is not mandatory to issue this command for all the species involved in a simulation. The species whose properties are not set with the `define_species_properties` command are reemitted when they interact with the structure and no reaction occurs.

Syntax

To specify the default event to be executed when a flux species hits a structure and no reaction occurs:

```
define_species_properties name=<c> species=<c> [default_event=<c>]
```

When simulating charge-up, you must specify the mass and charge of every flux species:

```
define_species_properties charge=<n> mass=<n> name=<c> species=<c> \
    [default_event=<c>]
```

Note:

The charge-up feature is switched on automatically when a charged flux species is defined by this command.

To specify the default event for a BCA reaction:

```
define_species_properties name=<c> species=<c> \
    [atomic_number=<n>] [bca_binding_energy=<n>] \
    [bca_electronic_stopping=<l>] \
    [bca_electronic_stopping_species=<l>] \
    [default_event=<c>] [mass_density=<n>] \
    [recombination_length=<n>]
```

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define_species_properties

In addition, when simulating charge-up, the electric properties of each material in the structure must be specified:

```
define_species_properties name=<c> species=<c> \
    [conductivity=<n>] [permittivity=<n>]
```

Note:

Any material with a nonzero conductivity is treated as an ideal conductor, that is, the value of the conductivity is not relevant for the electric field computation. A material with zero conductivity is treated automatically as a dielectric with the specified permittivity.

Table 55 Parameters of define_species_properties command

Parameter	Description
atomic_number	Sets the atomic number “Z” of the atom. Type: Number Default: none
bca_binding_energy	Sets the binding energy of a particle. As the cascade proceeds, any recoils that are near the surface, have a trajectory out of the structure, and have a kinetic energy that exceeds the binding energy will be emitted from the structure. Type: Number Default: 3.0 Unit: eV
bca_electronic_stopping	Sets the electronic stopping factor for each collision partner named in bca_electronic_stopping_species. For those not specified, the default value is used. For more information, see the <i>Sentaurus™ Process User Guide</i> , Nonlocal Electronic Stopping. The parameter name in Sentaurus Process is LSS.Pre. Type: List Default: 1.0
bca_electronic_stopping_species	Specifies a list of collision partners where the nondefault value of bca_electronic_stopping should be set. Type: List Default: none

Chapter 6: Input Commands

define_species_properties

Table 55 Parameters of *define_species_properties* command (Continued)

Parameter	Description
charge	Sets the charge of the species in units of the unit charge. Type: Number Default: 0 Range: (-∞, ∞) Unit: 1
conductivity	Sets the electrical conductivity of the species. By default, the species is treated as a dielectric (conductivity=0). Type: Number Default: 0 Range: [0, ∞) Unit: (Ωm) ⁻¹
default_event	Sets what happens to a molecule or an atom of the specified species when it interacts with the structure and no reaction occurs. Options are: <ul style="list-style-type: none">• discard• reemit For BCA reactions, it allows a BCA reaction to be set as the default event. The BCA reaction <code>incoming_species</code> must match this species. Type: Character Default: reemit; none for BCA reactions
mass	Sets the mass of the species. Type: Number Default: none Unit: amu (atomic mass units)
mass_density	Sets the density of a solid composed of this species. Type: Number Default: none Unit: kg/m ³
name	Sets the name used to refer to the species properties in a <code>define_etch_machine</code> command. Type: Character Default: none

Chapter 6: Input Commands

define_species_properties

Table 55 Parameters of define_species_properties command (Continued)

Parameter	Description
permittivity	Sets the relative permittivity (ϵ_r) of the medium. A species is treated as a dielectric only if it is nonconducting, that is, the value of this parameter is considered only if conductivity=0. Type: Number Default: 1 Range: (0, ∞) Unit: 1
recombination_length	For BCA target materials, this parameter sets the length below which vacancies and recoils recombine. Setting a value of 0 switches off recombination. The default is computed from the species mass and the material density (mass and mass_density parameters, respectively). Type: Number Default: $\left(\frac{\text{mass}}{\text{mass_density}}\right)^{\frac{1}{3}}$ Unit: m
species	Sets the name of the species for which the properties are defined. Type: Character Default: none

Species Used in BCA Reactions

BCA reactions require the specification of an atomic mass and an atomic number for all species involved in the reaction. In addition, the density and the binding energy of the target material (that is, the target_species parameter of the add_reaction command) must be specified. The binding energy, set with the binding_energy parameter, is the threshold energy above which particles with trajectories out the structure are considered to be sputtered.

You can specify target species for BCA reactions with either an “effective Z” or an “effective mass” and density, or you can define material replacements. In this case, the material particles are replaced with their component parts (that is, atoms that have Z, mass, and density defined) before the simulation begins. This is performed by specifying the split_replacements parameter of the etch or filter_structure command.

Chapter 6: Input Commands

define_species_properties

Examples

Define positively charged argon ions with a mass of 40 amu:

```
define_species_properties name=sp species=I mass=40 charge=1
```

Define a dielectric material with a relative electric permittivity of 11.7:

```
define_species_properties name=sp species=Silicon permittivity=11.7
```

Define a conducting material:

```
define_species_properties name=sp species=Aluminum \
conductivity=3.5e7
```

Chapter 6: Input Commands

define_structure

define_structure

This command defines a new structure. The structure can be loaded from a TDR boundary file, or it can be a cuboid (3D) or a rectangle (2D). For a PMC simulation, the structure can also be loaded from a PMC file or from a TDR file containing a 3D GC structure.

Note:

Multiple structures can be defined in the same input file, even of different dimensions. This allows you to mix 2D and 3D simulations in the same input file (see [Simulating Process Steps on 2D and 3D Structures on page 32](#)).

Syntax

To load a structure from a TDR file containing a boundary:

```
define_structure file=<c> [conformalize=<b>] [name=<c>] \
[read_fields=<b>] [slice_angle=<n>] [tdr_geometry=<c>] \
[tdr_geometry_search=<l>]
```

To load a structure from a TDR file containing a 3D GC structure:

```
define_structure file=<c> [name=<c>] [read_fields=<b>] \
[slice_angle=<n>] [tdr_geometry=<c>] [tdr_geometry_search=<l>]
```

To create a 3D cuboid or 2D rectangular structure from the beginning:

```
define_structure material=<c> point_max=<v> point_min=<v> \
[flat_orientation=<v>] [name=<c>] [read_fields=<b>] [region=<c>] \
[slice_angle=<n>] [vertical_orientation=<v>]
```

To load a PMC structure from a PMC file:

```
define_structure pmc_file=<c> \
[initial_structure_name=<c>] [name=<c>] [read_fields=<b>] \
[slice_angle=<n>]
```

Table 56 Parameters of define_structure command

Parameter	Description
conformalize	If true, an operation is performed to make input boundaries conformal. Type: Boolean Default: false
file	Sets the path of the TDR boundary file containing the structure. Type: Character Default: none

Chapter 6: Input Commands

define_structure

Table 56 Parameters of define_structure command (Continued)

Parameter	Description
flat_orientation	Sets the Miller index of the direction perpendicular to the wafer flat (y-axis of the wafer coordinate system) for the newly created region. Type: Vector Default: {1 1 0}
initial_structure_name	Sets a new name for the initial structure loaded from a PMC file and that can be used as the body of Boolean operations. Type: Character Default: none
material	Sets the material of the initial cube. Type: Character Default: none
name	Sets the name of the structure. Type: Character Default: default_structure
pmc_file	Sets the file name or path to a PMC file from which to load the initial data structure. Type: Character Default: none
point_max	Sets the maximum corner point of the initial cube. Type: Vector Default: none Unit: μm
point_min	Sets the minimum corner point of the initial cube. Type: Vector Default: none Unit: μm
read_fields	If true, then all vertex scalar data is read from the mixed-element geometry of the TDR file and is available to use in the field_names parameter of the define_material_replacement command (see define_material_replacement on page 285). Type: Boolean Default: false

Chapter 6: Input Commands

define_structure

Table 56 Parameters of define_structure command (Continued)

Parameter	Description
region	Sets the name of the created region if the structure is not loaded from a file. Type: Character Default: none
slice_angle	Sets the rotation of the x-axis of the simulation coordinate system with respect to the y-axis of the wafer coordinate system. Note: This parameter does not support the radian measurement unit. Type: Number Default: -90 Range: [-180, 180] Unit: degree
tdr_geometry	Sets the name of the geometry to load from the TDR file specified by file. A geometry with this name must exist in the specified TDR file. The geometries stored in the specified TDR file are searched in the order specified by parameter tdr_geometry_search. If tdr_geometry is not specified, then the first geometry type (as specified by tdr_geometry_search) present in the file is located and then the last geometry of that type is loaded. Type: Character Default: none
tdr_geometry_search	Specifies the order in which to locate a valid TDR geometry. Options are: <ul style="list-style-type: none">• brep• gc Note: The list must not be empty. Type: List Default: {brep gc}
vertical_orientation	Sets the Miller index of the direction perpendicular to the wafer surface (z-axis of the wafer coordinate system) for the newly created region. Type: Vector Default: {0 0 1}

Chapter 6: Input Commands

define_structure

Note:

To create a rectangle, the vector values of `point_min` and `point_max` must have two components. To create a cuboid, three components must be specified.

The Miller indices for a plane are usually written as `(hkl)`, and the set of equivalent planes is written as `{hkl}`. A crystal direction is usually written as `[hkl]`, and the set of equivalent directions is written as `<hkl>`. The value assigned to the parameters `flat_orientation` and `vertical_orientation` is a Tcl list of indices representing a crystal direction. The braces in the specified value are required to form a Tcl list and do not indicate a set of equivalent planes.

Examples

Example of conformal input:

```
define_structure file=input.tdr
```

This command imports a structure from the file `input.tdr`. The input is assumed to have conformal boundaries.

Note:

If multiple geometries are present and the `tdr_geometry` parameter is not specified, the last valid TDR boundary in the TDR file is selected automatically.

Example of loading a specific TDR geometry from a file:

```
define_structure file=input.tdr tdr_geometry="geometry_0"
```

This command imports the TDR geometry `geometry_0` from the file `input.tdr`, and it ignores all other geometries in the file. The input is assumed to have conformal boundaries.

Example of nonconformal input:

```
define_structure file=input.tdr conformalize=true \
    name=conformalized_input
```

This command imports a structure from the file `input.tdr`. An operation on the structure is performed to create conformal boundaries between regions. The name of the structure is `conformalized_input`.

Example of defining a 3D cuboid structure from the beginning:

```
define_structure material=Silicon point_max={1 1 1} \
    point_min={0 0 0} region="substrate"
```

This command creates an initial cuboid structure, with silicon as the material and `substrate` as the name of the region.

Chapter 6: Input Commands

define_structure

Example of defining a 2D rectangular structure from the beginning:

```
define_structure material=Silicon point_max={1 1} point_min={0 0}
```

This command creates an initial 2D rectangular structure, with silicon as the material.

Loading a PMC Structure

A PMC structure is loaded from a PMC file with the `define_structure` command when the parameter `pmc_file` is used.

When the PMC file contains an initial structure, it will be loaded. The parameter `initial_structure_name` can be used to rename the initial structure to the specified name. See [Saving PMC Structures on page 537](#).

Note:

A PMC file is not a TDR file and cannot be visualized with Sentaurus Visual. It can only be loaded in to Sentaurus Topography 3D.

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define_surface_transport_model

define_surface_transport_model

This command defines a surface transport model to specify the behavior of surface diffusing particles (see [Surface Transport Model on page 92](#)).

Syntax

```
define_surface_transport_model name=<c> \
    [collect_statistics=<b>] [max_num_events=<n>] [max_time=<n>]
```

Table 57 Parameters of *define_surface_transport_model* command

Parameter	Description
collect_statistics	Specifies whether to collect statistical data about the diffusion process to be plotted in the PMC statistics HTML report. Type: Boolean Default: none
max_num_events	Sets the maximum number of events to execute before the diffusing adatom is discarded. Type: Number Default: 10^8 Range: $[0, \infty[$
max_time	Sets the maximum physical time span in which an adatom can diffuse before it is discarded. Type: Number Default: ∞ Range: $[0, \infty[$ Unit: s
name	Sets the name of the surface transport model to be referenced in the <code>define_etch_machine</code> command and the <code>add_event</code> command. Type: Character Default: none

Examples

See [Surface Transport Model on page 92](#).

Chapter 6: Input Commands

define_volumetric_species_distribution

define_volumetric_species_distribution

This command defines the distribution of a volumetric source.

Note:

The defined volumetric distribution is energy-dependent only if `energy_max` and `energy_min` are specified.

Syntax

```
define_volumetric_species_distribution name=<c> \
    generation_rate=<c> species=<c> \
    [energy_max=<c> energy_min=<c>] [point_max=<v>] [point_min=<v>] \
    [sampling_time_step=<n>]
```

Table 58 Parameters of `define_volumetric_species_distribution` command

Parameter	Description
<code>energy_max</code>	Sets the expression of the maximum energy of the specified uniform energy distribution. Type: Character Default: 0 Range: Time-dependent expression, evaluating to $[0, \infty[$ and not smaller than the value of the time-dependent expression <code>energy_min</code> at the same time Unit: eV
<code>energy_min</code>	Sets the expression of the minimum energy of the specified uniform energy distribution. Type: Character Default: none Range: Time-dependent expression, evaluating to $[0, \infty[$ and not larger than the value of the time-dependent expression <code>energy_max</code> at the same time Unit: eV
<code>generation_rate</code>	Sets the time- and position-dependent expression for the number of molecules or atoms of the specified species generated per unit time and volume. For details about time- and position-dependent expressions, see Syntax for Expressions on page 139 . Type: Character Default: none Range: Time-dependent expression, evaluating to $[0, \infty[$ Unit: mol/m ³ /s

Chapter 6: Input Commands

define_volumetric_species_distribution

Table 58 Parameters of define_volumetric_species_distribution command (Continued)

Parameter	Description
name	Sets the name of the volumetric species distribution. Type: Character Default: none
point_max	Sets the requested maximum corner of the cuboid domain where particles will be generated. The generation rate of the particles will be zero outside of this cuboid domain. The actual maximum corner of the cuboid domain is obtained by snapping the point_max value to a grid point of the PMC structure used during the simulation Type: Vector Default: {∞ ∞ ∞} Unit: μm
point_min	Sets the requested minimum corner of the cuboid domain where particles will be generated. The generation rate of the particles will be zero outside of this cuboid domain. The actual minimum corner of the cuboid domain is obtained by snapping the point_min value to a grid point of the PMC structure used during the simulation. Type: Vector Default: {-∞ -∞ -∞} Unit: μm
sampling_time_step	Sets the smallest time step used to sample the time-dependent expression of generation_rate, energy_min, and energy_max. Note: This parameter is mandatory when the value of generation_rate, energy_min, or energy_max is a time-dependent expression. An expression is considered time dependent if it contains the t string. Otherwise, it is time independent. Type: Number Default: none Unit: minute
species	Sets the name of the species for which the distribution is defined. Type: Character Default: none

Chapter 6: Input Commands

define_yield

define_yield

This command specifies the properties of a new yield function that depends on the species of the incoming particles, its energy, and the target surface material. When defining a yield function for a machine using an RFM model, the value of the `species` parameter must be the name of an ion flux of that model.

As for ion distributions, Sentaurus Topography 3D supports collections of yield functions (see *Examples*).

This yield function can be used in RFM or reaction models that take sputtering into account.

Syntax

Define energy-dependent or energy-independent yield functions:

```
define_yield energy=<n> material=<c> name=<c> normalized=<b> \
    species=<c> table=<v> [angle_unit=<c>]

define_yield energy=<n> material=<c> name=<c> s1=<n> s2=<n> \
    species=<c> \
    [threshold_energy=<n>] [yield_at_zero=<n>]

define_yield energy=<n> material=<c> name=<c> species=<c> \
    sputtering=false

define_yield energy=<n> material=<c> name=<c> species=<c> \
    theta_max=<n> yield_max=<n> \
    [threshold_energy=<n>] [yield_at_zero=<n>]
```

Define two-part yield function:

```
define_yield (energy=<n> | threshold_energy=<n>) material=<c> \
    name=<c> sigma1=<n> sigma2=<n> species=<c> \
    theta_max=<n> yield_at_90=<n> \
    yield_at_zero=<n> yield_max=<n>
```

Define yield function using expression:

```
define_yield expression=<c> material=<c> name=<c> [energy=<n>]
```

Chapter 6: Input Commands

define_yield

Table 59 Parameters of define_yield command

Parameter	Description
angle_unit	Sets the unit of the angles listed in the table parameter. Options are: <ul style="list-style-type: none">• deg• rad Type: Character Default: deg
energy	Sets the energy for which the yield function is defined. When energy=0, the yield function is valid at all energies, that is, it is energy independent. Type: Number Default: none Range: [0, ∞[Unit: eV
expression	Sets the formula used to calculate the yield function. When you specify expression, the yield function is defined from the user-specified expression, and the energy parameter is optional. For details about energy- and angle-dependent expressions, see Syntax for Expressions on page 139 . There are the following cases: <ul style="list-style-type: none">• When energy is not specified, the specified expression defines an energy-dependent yield function that is valid for all energy levels.• When energy=0, the specified expression defines an energy-independent yield function.• When energy is set to a positive value, the specified expression defines the angle-dependent part of the yield function for the given energy level. Type: Character Default: none
material	Sets the name of the surface material for which the yield function is defined. Type: Character Default: none
name	Sets the name used to reference the yield function in a define_deposit_machine or define_etch_machine command. Type: Character Default: none

Chapter 6: Input Commands

define_yield

Table 59 Parameters of define_yield command (Continued)

Parameter	Description
normalized	Specifies whether the value of the yield function at 0° must be 1 (normalized=true) or whether it can be any nonnegative value (normalized=false). Type: Boolean Default: none
s1	Sets the first sputter coefficient. Type: Number Default: none
s2	Sets the second sputter coefficient. Type: Number Default: none
sigma1	Sets the angular spread for the lower part of a two-part yield model. Type: Number Default: none Range: [0, 90] Unit: degree
sigma2	Sets the angular spread for the upper part of a two-part yield model. Type: Number Default: none Range: [0, 90] Unit: degree
species	Sets the name of the flux species for which the yield function is defined. Type: Character Default: none
sputtering	When sputtering=false for a certain species and material pair, sputtering by particles of that species from that material is deactivated completely. The only option is sputtering=false. Type: Boolean Default: none

Chapter 6: Input Commands

define_yield

Table 59 Parameters of define_yield command (Continued)

Parameter	Description
table	<p>Sets the tabular format of the yield function.</p> <p>Values of the yield function are specified in a tabular form similar to the ion angular distribution (IAD), where the first column represents angles and the second column is the value of the yield function. The restrictions on the format of the table are the same as for the <code>define_iad</code> command (see define_iad on page 274).</p> <p>In addition, if <code>normalized=true</code>, then the value of the yield function for 0° must be exactly 1.</p> <p>Type: Vector</p> <p>Default: none</p>
theta_max	<p>Sets the angle at which the yield function has its maximum.</p> <p>Type: Number</p> <p>Default: none</p> <p>Range: $[0, 90]$</p> <p>Unit: degree</p>
threshold_energy	<p>When this parameter is specified, the yield function becomes energy dependent (see Equation 88).</p> <p>This parameter cannot be used with the <code>energy</code>, <code>expression</code>, or <code>table</code> parameters.</p> <p>Type: Number</p> <p>Default: 0</p> <p>Unit: eV</p>
yield_at_90	<p>Sets the value of the yield function at the grazing incidence.</p> <p>Type: Number</p> <p>Default: 0</p> <p>Range: $[0, \infty[$</p>
yield_at_zero	<p>Sets the value of the yield function at normal incidence.</p> <p>Type: Number</p> <p>Default: 1</p> <p>Range: $[0, \infty[$ (when <code>s1</code> and <code>s2</code> are used) $(0, \infty[$ (when <code>theta_max</code> and <code>yield_max</code> are used)</p>
yield_max	<p>Sets the maximum value of the yield function.</p> <p>Type: Number</p> <p>Default: none</p> <p>Range: $[1, \infty[$</p>

Chapter 6: Input Commands

define_yield

Description

You can define yield functions distinctly in each combination of species and material. Yield functions are naturally angle dependent. There are different ways to handle energy dependence of yield:

- **Energy independent:** Set `energy=0` to specify that a yield function is valid at all energies.
- **Linear interpolation:** Specify a yield function for at least two different energy levels. The lowest energy specified is the threshold energy for the yield function. For ion energy values that have not been specified, the value of the yield function is calculated by linearly interpolating the parameter values for analytic yield functions or the specified values for tabular yield functions.
- **Energy dependent:** Specify the `threshold_energy` parameter, which cannot be used with the `energy` parameter, so that the built-in yield function becomes energy dependent as follows:

$$\gamma(\theta, E) = (\sqrt{E} - \sqrt{E_{\text{th}}})\gamma(\theta) \quad (88)$$

where E_{th} represents the value of the `threshold_energy` parameter.

- **Energy-dependent expression:** Specify expressions containing E to define a custom energy-dependent yield function.

Note:

Energy-dependent yield functions can be used only with reaction models, not with level set-based models.

When you specify the parameters `s1` and `s2`, the yield function is defined as:

$$\gamma(\theta) = \gamma_0(s_1 \cos \theta + s_2 \cos^2 \theta + (1 - s_1 - s_2) \cos^4 \theta) \quad (89)$$

where γ_0 denotes the value of the `yield_at_zero` parameter.

When you specify the parameters `theta_max` and `yield_max`, the yield function is defined as [15]:

$$\gamma(\theta) = \gamma_0 \cos^{-f} \theta \exp(-s(1/\cos \theta - 1)) \quad (90)$$

where $f = -\ln(\gamma_{\text{max}}/\gamma_0)/(\ln(\cos(\theta_{\text{max}})) + 1 - \cos \theta_{\text{max}})$ and $s = f \cos \theta_{\text{max}}$.

When you specify `sigma1`, `sigma2`, `theta_max`, `yield_at_zero`, `yield_at_90`, and `yield_max`, you obtain a two-part yield function, which is given by:

$$\gamma(\theta) = \begin{cases} \gamma_l(\theta), & \theta < \theta_{\text{max}} \\ \gamma_u(\theta), & \theta \geq \theta_{\text{max}} \end{cases} \quad (91)$$

Chapter 6: Input Commands

define_yield

where:

$$\gamma_l(\theta) = \gamma_0 + (\gamma_{\max} - \gamma_0) \left[e^{-\frac{1}{2}\left(\frac{\theta_{\max} - \theta}{\sigma_1}\right)^2} - e^{-\frac{1}{2}\left(\frac{\theta_{\max}}{\sigma_1}\right)^2} \right] \quad (92)$$

$$\gamma_u(\theta) = \gamma_{90} + (\gamma_{\max} - \gamma_{90}) \left[e^{-\frac{1}{2}\left(\frac{\theta - \theta_{\max}}{\sigma_2}\right)^2} - e^{-\frac{1}{2}\left(\frac{90 - \theta_{\max}}{\sigma_2}\right)^2} \right] \quad (93)$$

and where:

- σ_1, σ_2 represent the values of the `sigma1` parameter and `sigma2` parameter, respectively.
- θ_{\max} represents the value of the `theta_max` parameter.
- γ_{90} represents the value of the `yield_at_90` parameter.
- γ_0 represents the value of the `yield_at_zero` parameter.
- γ_{\max} represents the value of the `yield_max` parameter.
- The angles θ and θ_{\max} are measured in degrees.

Examples

Define an energy-independent yield function for silicon sputtering from species Ar that is proportional to the cosine of the angle between the direction of the impinging particle and the surface normal at the collision point:

```
define_yield name=my_yield species=Ar material=Silicon energy=0 \
expression="0.3*cos(theta)"
```

Define an energy-dependent yield function for silicon sputtering from species Ar that is equal to zero when the energy of the impinging particle is smaller than 85 eV and that is proportional to the cosine of the angle between the direction of the impinging particle and the surface normal at the collision point, otherwise:

```
define_yield name=my_yield species=Ar material=Silicon \
expression="E >= 85.0 ? 0.3*cos(theta) : 0."
```

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define_yield

Define a collection of energy-independent yield functions called `my_yield` for flux `I` and several target materials:

```
define_yield name=my_yield species=I energy=0 material=Silicon \
    theta_max=55 yield_max=1.5

define_yield name=my_yield species=I energy=0 material=Oxide s1=6.0 \
    s2=-5.5

define_yield name=my_yield species=I energy=0 material=Nitride \
    theta_max=60 yield_max=1.75

define_yield name=my_yield species=I energy=0 material=Photoresist \
    table=$yield_table
```

Chapter 6: Input Commands

deposit

deposit

This command starts a deposition simulation either by using a machine defined using the `define_deposit_machine` command or by geometrically depositing a shape defined by the `define_shape` command.

Syntax

Deposition simulation on the surface of a structure using a machine:

```
deposit (cycles=<n> | time=<n>) spacing=<v> \
[accuracy=<n>] [cfl=<n>] [comment=<c>] [decimate=<b>] \
[diffusion_flux_error_control_strategy=<c>] \
[diffusion_flux_integration_error=<n>] [engine=<c>] \
[exposed_only=<b>] \
[extraction=<c> (extraction_interval=<n> | \
extraction_times=<v> [extraction_times_unit=<c>]) \
[extraction_file_update_interval=<n>] \
[force_intermediate_extraction=<b>]] \
[file=<c>] [flat_orientation=<v>] \
[integration_error=<n> | integration_samples=<n>] \
[machine=<c>] [max_ion_reflections=<n>] [merge=<b>] \
[min_angle=<n>] [min_dihedral_angle=<n>] \
[min_ion_reflection_probability=<n>] \
[(plot_interval=<n> [compute_first_plot=<b>] \
[compute_last_plot=<b>] | plot_times=<v> [plot_times_unit=<c>]) \
[force_intermediate_plot=<b>] [plot_file_update_interval=<n>] \
[plot_type=<l>] [split_plots=<b>]] \
[random_seed=<n>] [region=<c>] [remove_spurious_parts=<b>] \
[ridge_angle=<n>] [shortest_edge=<n>] \
[stop_plane=<n> | stop_point=<w>] \
[structure=<c>] [surface_accuracy=<n>] [surface_decimate=<b>] \
[surface_min_angle=<n>] [surface_min_dihedral_angle=<n>] \
[surface_ridge_angle=<n>] [surface_shortest_edge=<n>] \
[update_scheme=<c>] \
[variance_reduction=<c>] [vertical_orientation=<v>]
```

Geometric deposition using a shape:

On a boundary structure:

```
deposit material=<c> shape=<c> \
[accuracy=<n>] [comment=<c>] [decimate=<b>] [flat_orientation=<v>] \
[merge=<c>] [min_angle=<n>] [min_dihedral_angle=<n>] [region=<c>] \
[ridge_angle=<n>] [shortest_edge=<n>] [structure=<c>] \
[vertical_orientation=<v>]
```

On a PMC structure:

```
deposit material=<c> shape=<c> [comment=<c>] [structure=<c>]
```

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deposit

Table 60 Parameters of deposit command

Parameter	Description
accuracy	<p>Sets the maximum deviation between the decimated surface of the boundary structure produced by Boolean operations and its original surface.</p> <p>When set to -1, the used value is half of the structure-dependent spacing epsilon¹.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none"> • The <code>structure</code> parameter denotes a boundary structure. • You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_accuracy=<n></code> Range: {-1} \cup [0, ∞[Unit: μm</p>
cfl	<p>Sets the Courant–Friedrichs–Lowy (CFL) number [16] for the integration of the surface evolution equation.</p> <p>Type: Number Default: 0.95 (when using a machine having <code>model=simple</code>) 0.5 (when using a machine not having <code>model=simple</code>) Range:]0, 1]</p>
comment	<p>Sets a comment for this process step that will be displayed or written to the log file.</p> <p>Type: Character Default: empty string</p>
compute_first_plot	<p>When <code>plot_interval</code> is set, the parameter <code>compute_first_plot</code> specifies whether to produce an intermediate plot at <code>time=0</code>.</p> <p>Type: Boolean Default: <code>true</code></p>
compute_last_plot	<p>When <code>plot_interval</code> is set, the parameter <code>compute_last_plot</code> specifies whether to produce an intermediate plot at the end of the simulation.</p> <p>Type: Boolean Default: <code>true</code></p>

Chapter 6: Input Commands

deposit

Table 60 Parameters of deposit command (Continued)

Parameter	Description
cycles	Sets the number of deposition cycles for a machine using the <code>ald</code> model. Type: Number Default: none Range: [0, 2147483647]
decimate	Specifies whether to decimate the boundary structure produced by Boolean operations. It can be specified only if structure denotes a boundary structure. Type: Boolean Default: Value set by <code>let decimate=</code>
diffusion_flux_error_control_strategy	Sets which type of error the parameter <code>diffusion_flux_integration_error</code> calculates. Options are: <ul style="list-style-type: none"> • <code>absolute</code>: Absolute error. • <code>relative</code>: Relative error. Type: Character Default: relative
diffusion_flux_integration_error	Sets the requested flux error of the diffusing species. Type: Number Default: 0.05 Range: [0, 1]
engine	Sets the engine to use for flux computation. This choice is available only for flux models. Options are: <ul style="list-style-type: none"> • <code>monte_carlo</code> • <code>radiosity</code> Type: Character Default: radiosity
exposed_only	Specifies whether deposition is possible only on exposed portions of the surface when using the <code>simple</code> model. Type: Boolean Default: false
extraction	Sets the name of the group of extractions to run during this process step. Type: Character Default: none

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deposit

Table 60 Parameters of deposit command (Continued)

Parameter	Description
extraction_file_update_interval	<p>Sets the time interval after which intermediate extraction results are written to file.</p> <p>When set to 0, intermediate extraction results are written to file immediately after they are created.</p> <p>Note: This parameter can be set only when at least one intermediate extraction produces file output.</p> <p>Type: Number Default: 0 Range: $[0, \infty[$ Unit: minute</p>
extraction_interval	<p>Sets the process time interval after which intermediate extractions must be executed.</p> <p>Type: Number Default: none Range: $]0, \infty[$ Unit: minute</p>
extraction_times	<p>Sets the times at which to perform intermediate extractions.</p> <p>The given vector must:</p> <ul style="list-style-type: none"> Contain only nonnegative values Be sorted in ascending order Contain no value larger than the value of parameter time <p>If any of these conditions is not met, then an error is issued.</p> <p>Type: Vector Default: none</p>
extraction_times_unit	<p>Sets the unit of the extraction_times values. Options are:</p> <ul style="list-style-type: none"> s (seconds) min (minutes) <p>Type: Character Default: min</p>

Chapter 6: Input Commands

deposit

Table 60 Parameters of deposit command (Continued)

Parameter	Description
file	Sets the file name into which intermediate surfaces and surface data should be saved. Used in conjunction with plot_interval only. In the file name, <base_name> denotes the value of the base_name parameter of the let command. Type: Character Default: <base_name>.tdr
flat_orientation	Sets the Miller index of the direction perpendicular to the wafer flat (y-axis of the wafer coordinate system) for the newly created region. It can be specified only if structure denotes a boundary structure. Type: Vector Default: {1 1 0}
force_intermediate_extraction	Specifies whether to compute intermediate extractions and, if applicable, write them to files even if Sentaurus Topography 3D was started with the command-line option --no_intermediate_extraction. Type: Boolean Default: false
force_intermediate_plot	Specifies whether to compute intermediate plots and write them to files even if Sentaurus Topography 3D was started with the --no_intermediate_plot command-line option. Type: Boolean Default: false
integration_error	Sets the maximum relative discretization error in the direct flux calculation. Type: Number Default: 0.05 Range:]0, 1]

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deposit

Table 60 Parameters of deposit command (Continued)

Parameter	Description
integration_samples	<p>Sets the number of integration points in the numeric integration.</p> <p>The meaning of this parameter depends on the value of the engine parameter:</p> <ul style="list-style-type: none"> • When engine=radiosity, integration_samples describes the number of discretization points, per surface element, in the hemisphere where visibility is determined. • When engine=monte_carlo, integration_samples describes the number of particle paths, per surface element, used in the flux integration. <p>Note: This parameter is deprecated for engine=radiosity. Instead, use the parameter integration_error.</p> <p>Type: Number Default: 1000 (engine= radiosity) 700 (engine=monte_carlo and variance_reduction=M-2016.12) 350 (engine=monte_carlo and variance_reduction=N-2017.09) Range: [1, ∞[</p>
machine	<p>Sets the name of the machine that is used for the deposition process.</p> <p>Type: Character Default: default_machine</p>
material	<p>Sets the material to be deposited.</p> <p>Type: Character Default: none</p>
max_ion_reflections	<p>Sets the maximum number of ion reflections to compute during flux integration. The specified value must be an integer. Only applicable when using RFM models.</p> <p>Type: Number Default: 1 Range: [1, ∞[</p>

Chapter 6: Input Commands

deposit

Table 60 Parameters of deposit command (Continued)

Parameter	Description
merge	If true, the deposited region merges with the already existing regions of the same material in the structure. It can be specified only if structure denotes a boundary structure. Type: Boolean Default: false
min_angle	Sets the smallest angle in the elements of the decimated surface of the boundary structure produced by Boolean operations. This parameter can be specified only if all of the following conditions are met: <ul style="list-style-type: none"> The structure parameter denotes a boundary structure. You specify decimate=true or, if you do not specify decimate, you did not specify let decimate=false. Type: Number Default: Value set by let decimate_min_angle=<n> Range: [0, 180] Unit: degree
min_dihedral_angle	Sets the smallest dihedral angle between two elements of the decimated surface of the boundary structure produced by Boolean operations that share an edge. This parameter can be specified only if all of the following conditions are met: <ul style="list-style-type: none"> The structure parameter denotes a boundary structure. You specify decimate=true or, if you do not specify decimate, you did not specify let decimate=false. Type: Number Default: Value set by let decimate_min_dihedral_angle=<n> Range: [0, 180] Unit: degree
min_ion_reflection_probability	Sets the threshold for the reflection probability below which multiple reflection is stopped. Type: Number Default: 0.001 Range: [0, 1]

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deposit

Table 60 Parameters of deposit command (Continued)

Parameter	Description
plot_file_update_interval	<p>Sets the time interval after which intermediate plots are written to file. When set to 0, intermediate plots are written to file immediately after they are created.</p> <p>Note: This parameter can be set only when <code>split_plots=false</code>.</p> <p>Type: Number Default: 0 Range: $[0, \infty[$ Unit: minute</p>
plot_interval	<p>Sets the process time interval after which intermediate exposed surfaces and surface data should be plotted. See TDR Dataset Names for Fluxes on page 390.</p> <p>Type: Number Default: none Range: $[0, \infty[$ Unit: minute</p>
plot_times	<p>Sets the times at which to perform intermediate plots. The given vector must:</p> <ul style="list-style-type: none">Contain only nonnegative valuesBe sorted in ascending orderContain no value larger than the value of parameter <code>time</code> <p>If any of these conditions is not met, then an error is issued.</p> <p>Type: Vector Default: none</p>
plot_times_unit	<p>Sets the unit of the <code>plot_times</code> values. Options are:</p> <ul style="list-style-type: none">s (seconds)min (minutes) <p>Type: Character Default: min</p>

Chapter 6: Input Commands

deposit

Table 60 Parameters of deposit command (Continued)

Parameter	Description
plot_type	<p>Sets the data type to save at the time intervals specified by <code>plot_interval</code>. Options are:</p> <ul style="list-style-type: none"> • <code>structure</code>: Saves multiregion boundary. • <code>surface</code>: Saves exposed surface with datasets. <p>Type: List Default: <code>surface</code></p>
random_seed	<p>Sets the seed of the pseudo-random number generator used by the Monte Carlo flux integrator.</p> <p>Note: This parameter can be specified only when <code>engine=monte_carlo</code>.</p> <p>Type: Number Default: 1 Range: [1, 2147483647]</p>
region	<p>Sets the name of the region that is deposited. It can be specified only if <code>structure</code> denotes a boundary structure.</p> <p>Type: Character Default: none</p>
remove_spurious_parts	<p>Specifies whether or not to remove spurious parts after running the process step.</p> <p>Type: Boolean Default: false</p>
ridge_angle	<p>Sets the angle used by the decimation algorithm to determine geometric features of the boundary structure produced by Boolean operations.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none"> • The <code>structure</code> parameter denotes a boundary structure. • You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_ridge_angle=<n></code> Range: [0, 180] Unit: degree</p>

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deposit

Table 60 Parameters of deposit command (Continued)

Parameter	Description
shape	Sets the name of the shape that is used for the deposition process. Type: Character Default: none
shortest_edge	Sets the shortest edge of the decimated surface of the boundary structure produced by Boolean operations. When set to -1, the used value is half of the structure-dependent spacing epsilon ¹ . This parameter can be specified only if all of the following conditions are met: <ul style="list-style-type: none"> The structure parameter denotes a boundary structure. You specify decimate=true or, if you do not specify decimate, you did not specify let decimate=false. Type: Number Default: Value set by let decimate_shortest_edge=<n> Range: {-1} ∪ [0, ∞[Unit: μm
spacing	Sets the cell size of the grid used to compute the surface evolution for each dimension. A vector with only one component can be used to set the grid cell size to the same value for all dimensions. For a machine using any model other than spin_on, for 2D and 3D structures, a vector with two and three components, respectively, can be used to specify the grid cell size separately for each dimension. For a machine using the spin_on model, for 3D structures, a vector with two components can be used to specify the grid cell size separately for each dimension. See Discretization Size and Accuracy on page 26 . Type: Vector Default: none Unit: μm
split_plots	Specifies whether to write intermediate plots each to a different file. Type: Boolean Default: false

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deposit

Table 60 Parameters of deposit command (Continued)

Parameter	Description
stop_plane	Sets the vertical coordinate of a horizontal plane above the exposed surface. When the exposed surface reaches or crosses this plane, time-stepping stops. See Stopping Time-Stepping on page 389 . Type: Number Default: none Unit: μm
stop_point	Specifies a list of coordinates of points above the exposed surface. When the exposed surface reaches or crosses any of these points, the simulation stops. See Stopping Time-Stepping on page 389 . Type: Vector list Default: none Unit: μm
structure	Sets the name of the structure on which deposition will occur. Type: Character Default: default_structure
surface_accuracy	Sets the maximum deviation between the decimated exposed surface and the original exposed surface. When set to -1, the used value is half of the structure-dependent spacing epsilon ¹ . It can be specified only if surface_decimate=true, or if you do not specify the surface_decimate parameter and specify let surface_decimate=true. Type: Number Default: Value set by let surface_decimate_accuracy=<n> Range: {-1} \cup [0, ∞ [Unit: μm
surface_decimate	Specifies whether to decimate the exposed surface used as an operand of Boolean operations. Type: Boolean Default: Value set by let surface_decimate=

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deposit

Table 60 Parameters of deposit command (Continued)

Parameter	Description
surface_min_angle	<p>Sets the smallest angle in the elements of the decimated exposed surface used as an operand of Boolean operations.</p> <p>It can be specified only if <code>surface_decimate=true</code>, or if you do not specify the <code>surface_decimate</code> parameter and specify <code>let surface_decimate=true</code>.</p> <p>Type: Number Default: Value set by <code>let surface_decimate_min_angle=<n></code> Range: [0, 180] Unit: degree</p>
surface_min_dihedral_angle	<p>Sets the smallest dihedral angle between two elements, which share an edge, of the decimated exposed surface used as an operand of Boolean operations.</p> <p>It can be specified only if <code>surface_decimate=true</code>, or if you do not specify the <code>surface_decimate</code> parameter and specify <code>let surface_decimate=true</code>.</p> <p>Type: Number Default: Value set by <code>let surface_decimate_min_dihedral_angle=<n></code> Range: [0, 180] Unit: degree</p>
surface_ridge_angle	<p>Sets the angle used by the decimation algorithm to determine geometric features of the exposed surface used as an operand of Boolean operations.</p> <p>It can be specified only if <code>surface_decimate=true</code>, or if you do not specify the <code>surface_decimate</code> parameter and specify <code>let surface_decimate=true</code>.</p> <p>Type: Number Default: Value set by <code>let surface_decimate_ridge_angle=<n></code> Range: [0, 180] Unit: degree</p>

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deposit

Table 60 Parameters of deposit command (Continued)

Parameter	Description
surface_shortest_edge	<p>Sets the shortest edge of the decimated exposed surface used as an operand of Boolean operations.</p> <p>When set to -1, the used value is half of the structure dependent spacing epsilon¹.</p> <p>It can be specified only if <code>surface_decimate=true</code>, or if you do not specify the <code>surface_decimate</code> parameter and specify <code>let surface_decimate=true</code>.</p> <p>Type: Number</p> <p>Default: Value set by <code>let surface_decimate_shortest_edge=<n></code></p> <p>Range: {-1} \cup [0, ∞[</p> <p>Unit: μm</p>
time	<p>Sets the simulation time.</p> <p>Type: Number</p> <p>Default: none</p> <p>Unit: minute</p>
update_scheme	<p>Sets the update scheme for the time integration of the level-set function. Options are:</p> <ul style="list-style-type: none"> • lax_friedrichs • upwind <p>Type: Character</p> <p>Default: upwind</p>
variance_reduction	<p>Sets the algorithm to use for variance reduction by the Monte Carlo flux integrator. Options are:</p> <ul style="list-style-type: none"> • N-2017.09 • M-2016.12 <p>Type: Character</p> <p>Default: N-2017.09</p>
vertical_orientation	<p>Sets the Miller index of the direction perpendicular to the wafer surface (z-axis of the wafer coordinate system) for the newly created region. It can be specified only if <code>structure</code> denotes a boundary structure.</p> <p>Type: Vector</p> <p>Default: {0 0 1}</p>

1. The structure-dependent spacing epsilon is logged out when defining a structure using the `define_structure` command.

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Note:

The Miller indices for a plane are usually written as (hkl), and the set of equivalent planes is written as {hkl}. A crystal direction is usually written as [hkl], and the set of equivalent directions is written as <hkl>. The value assigned to the parameters flat_orientation and vertical_orientation is a Tcl list of indices representing a crystal direction. The braces in the specified value are required to form a Tcl list and do not indicate a set of equivalent planes.

Limitations

The following limitations apply:

- The parameter structure cannot specify a PMC structure. To process such a structure, an explicit conversion of the structure is needed before calling the deposit command (see [Integration With Other Sentaurus Topography 3D Functionality on page 580](#)).
- When using a machine having model=crystal, the following parameters are not supported:

cfl, compute_first_plot, compute_last_plot, extraction_interval, extraction_times, extraction_times_unit, file, merge, plot_interval, plot_times, plot_times_unit, plot_type, stop_plane, stop_point, update_scheme

- The stop_plane, stop_point, and update_scheme parameters are not supported when using a machine having model=spin_on.
- For machines having model=spin_on, structures whose exposed surface cannot be described as a single-valued function of the x- and y-coordinates in three dimensions, or of the x-coordinate in two dimensions, are not supported. However, topologically connected exposed surfaces containing elements parallel to the vertical direction are supported.

Examples

Deposition process using a machine:

```
deposit machine=depomachine spacing={0.05 0.3 0.05} time=0.5
```

This command simulates a deposition process on the structure, using the machine depomachine with a grid spacing of dx=0.05 μm, dy=0.3 μm, dz=0.05 μm, and a simulation time of 0.5 minutes.

Note:

The resolution is adjusted internally to match the actual structure.

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Deposition process using a shape:

```
deposit shape=shape_1 material=Oxide comment="deposit shape"
```

This command deposits the shape `shape_1` onto the structure. The created region will consist of the material `Oxide`. The comment for this process step is displayed in the log file.

Note:

Parts of `shape_1` that overlap the existing structure are not added.

Deposition process with intermediate surface plotting:

```
deposit machine=depomachine spacing={0.1} time=0.5 \
    file=depo_surfaces.tdr plot_interval=0.1
```

This command deposits using the machine `depomachine`, with a grid spacing of $dx=dy=dz=0.1 \mu\text{m}$. Intermediate surfaces along with data such as surface velocities and fluxes are plotted into the file `depo_surfaces.tdr`. The surface of the first and last time steps of the simulation will always be plotted. During the simulation, whenever the simulation time surpasses an integral multiple of `plot_interval` (for example, 0.1, 0.2, 0.3...), a surface will be plotted to the file. This feature can check process parameters and model behavior.

Stopping Time-Stepping

The `stop_plane` and `stop_point` parameters of the `deposit` command allow you to stop time-stepping when a specified plane or point has been reached before the final process time.

These parameters can be used when processing both 2D and 3D structures.

The dimensions of the points specified with `stop_point` must match the dimensions of the structure for which it is used.

The values specified with `stop_plane` and `stop_point` must fulfill certain constraints with respect to the computational domain and the initial exposed surface.

The computational domain and the initial exposed surface are defined in [Boundary Types on page 31](#):

- When using `stop_plane`, the specified plane must intersect the computational domain, and the specified plane must be above the initial exposed surface.
- When using `stop_point`, the specified point must be inside the computational domain, and the specified point must lie above the initial exposed surface.

Due to the discrete time steps, the exposed surface can cross the specified plane or point in the last time step. The maximum distance of the final exposed surface beyond the specified

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plane or point is limited by the value of the parameter `spacing` that specifies the discretization of the level-set grid.

When using `stop_plane` or `stop_point`, the output written to the log file indicates why the time-stepping of the corresponding process step stopped.

If the specified plane or point was reached or crossed, the output indicates this. The output includes the specified plane or point and the process time at which this occurred. For example:

```
Exiting loop early: stop_plane= <> [um] has been reached at t=<>.
```

```
Exiting loop early: stop_point= {} [um] has been reached at t=<>.
```

If the specified plane or point is not reached or crossed, this is indicated in the output together with the specified plane or point and the specified process time. For example:

```
stop_plane= <> [um] has not been reached at any time step within  
time=<> [min].
```

```
stop_point= {} [um] has not been reached at any time step within  
time=<> [min].
```

Examples

Specify a stop plane for deposition on a 2D or 3D structure:

```
deposit spacing=0.1 time=1.0 stop_plane=1.0
```

Specify a stop point for deposition on a 3D structure:

```
deposit spacing=0.1 time=1.0 stop_point={0.0 0.5 0.3}
```

Specify a stop point for deposition on a 2D structure:

```
deposit spacing=0.1 time=1.0 stop_point={0.0 0.5}
```

TDR Dataset Names for Fluxes

For models that calculate ion or neutral fluxes, the values of the fluxes are written to TDR datasets when using the parameter `plot_interval`.

The name of a flux dataset starts with the name of the flux species. If the flux takes a yield function into account, it is followed by `yield`.

The type of flux is indicated by one of the following suffixes:

`direct` The direct flux that arrives from the plasma at a surface element.

`reactive` The incoming flux at a surface element that is available for reemission.

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- reflected** The direct flux that has been reflected away from a surface element.
- reflection** The incoming flux at a surface element that has been reflected from other surface elements.
- total** Sum of the reactive flux and the incoming indirect flux caused by the reactive flux.

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diffuse

This command performs a surface diffusion and convection step using physical parameters defined in the `define_diffuse_machine` command (see [define_diffuse_machine on page 234](#)).

Syntax

```
diffuse machine=<c> \
[accuracy=<n>] [cfl=<n>] [comment=<c>] [decimate=<b>] \
[field_files=<l>] [field_times=<l>] [file=<c>] \
[min_angle=<n>] [min_dihedral_angle=<n>] \
[force_intermediate_plot=<b>] \
[plot_interval=<n> [compute_first_plot=<b>]] \
[plot_times=<v> [plot_times_unit=<c>]) \
[plot_type=<c>] [ridge_angle=<n>] \
[shortest_edge=<n>] [spacing=<n>] [split_plots=<b>] \
[structure=<c>] [surface_accuracy=<n>] [surface_decimate=<c>] \
[surface_min_angle=<n>] [surface_min_dihedral_angle=<n>] \
[surface_shortest_edge=<n>] \
[temperature=<c>] [time=<c>]
```

Table 61 Parameters of diffuse command

Parameter	Description
accuracy	<p>Sets the maximum deviation between the decimated surface of the boundary structure produced by Boolean operations and its original surface.</p> <p>When set to <code>-1</code>, the used value is half of the structure-dependent spacing <code>epsilon</code>¹.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none">• The <code>structure</code> parameter denotes a boundary structure.• You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_accuracy=<n></code> Range: $\{-1\} \cup [0, \infty[$ Unit: μm</p>
cfl	<p>Sets the Courant–Friedrichs–Lowy (CFL) number [16] for the integration of the surface evolution equation.</p> <p>Type: Number Default: 0.95 (when using a machine having <code>model=simple</code>) 0.5 (when using a machine having not having <code>model=simple</code>) Range:]0, 1]</p>

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Table 61 Parameters of diffuse command (Continued)

Parameter	Description
comment	Sets a comment for this process step that is displayed or written to the log file. Type: Character Default: empty string
compute_first_plot	When <code>plot_interval</code> is set, the parameter <code>compute_first_plot</code> specifies whether to produce an intermediate plot at <code>time=0</code> . Type: Boolean Default: true
decimate	Specifies whether to decimate the boundary structure produced by Boolean operations. It can be specified only if <code>structure</code> denotes a boundary structure. Type: Boolean Default: Value set by <code>let decimate=</code>
field_files	Specifies a list of TDR files containing fields specified by the <code>fields</code> parameter of the <code>define_diffuse_machine</code> command. The particular machine is specified by the <code>machine</code> parameter. Interpolation in time and space is used to obtain values on the evolving surface. Use the <code>field_times</code> parameter to set the time corresponding to each TDR file. Type: List Default: none
field_times	Specifies an ordered list of the simulation times corresponding to the TDR files listed in <code>field_files</code> . The first in the list must be 0, and the last should be the same as the <code>time</code> parameter, and the rest should be in increasing order. Type: List Default: none Unit: s
file	Sets the file into which intermediate surfaces and surface data should be saved. Used in conjunction with <code>plot_interval</code> only. In the file name, <code><base_name></code> denotes the value of the <code>base_name</code> parameter of the <code>let</code> command. Type: Character Default: <code><base_name>.tdr</code>

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diffuse

Table 61 Parameters of diffuse command (Continued)

Parameter	Description
force_intermediate_plot	<p>Specifies whether to compute intermediate plots and write them to files even if Sentaurus Topography 3D was started with the <code>--no_intermediate_plot</code> command-line option.</p> <p>Type: Boolean Default: false</p>
machine	<p>Sets the name of the machine that is used for the diffusion process.</p> <p>Type: Character Default: default_machine</p>
min_angle	<p>Sets the smallest angle in the elements of the decimated surface of the boundary structure produced by Boolean operations.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none"> • The <code>structure</code> parameter denotes a boundary structure. • You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_min_angle=<n></code> Range: [0, 180] Unit: degree</p>
min_dihedral_angle	<p>Sets the smallest dihedral angle between two elements of the decimated surface of the boundary structure produced by Boolean operations that share an edge.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none"> • The <code>structure</code> parameter denotes a boundary structure. • You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_min_dihedral_angle=<n></code> Range: [0, 180] Unit: degree</p>

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diffuse

Table 61 Parameters of diffuse command (Continued)

Parameter	Description
plot_interval	Sets the process time interval after which intermediate exposed surfaces and surface data must be plotted. See TDR Dataset Names for Fluxes on page 429 . Type: Number Default: none Range: [0 , ∞ [Unit: minute
plot_times	Sets the times at which to create intermediate plots. The given vector must: <ul style="list-style-type: none"> Contain only nonnegative values Be sorted in ascending order Contain no value larger than the value of parameter <code>time</code> If any of these conditions is not met, then an error is issued. Type: Vector Default: none
plot_times_unit	Sets the unit of the <code>plot_times</code> values. Options are: <ul style="list-style-type: none"> s (seconds) min (minutes) Type: Character Default: min
plot_type	Specifies the type of intermediate plot. The only option is <code>surface</code> . Type: Character Default: none Range: surface
ridge_angle	Sets the angle used by the decimation algorithm to determine geometric features of the boundary structure produced by Boolean operations. This parameter can be specified only if all of the following conditions are met: <ul style="list-style-type: none"> The <code>structure</code> parameter denotes a boundary structure. You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. Type: Number Default: Value set by <code>let decimate_ridge_angle=<n></code> Range: [0 , 180] Unit: degree

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Table 61 Parameters of diffuse command (Continued)

Parameter	Description
shortest_edge	<p>Sets the shortest edge of the decimated surface of the boundary structure produced by Boolean operations.</p> <p>When set to -1, the used value is half of the structure-dependent spacing epsilon¹.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none"> The <code>structure</code> parameter denotes a boundary structure. You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_shortest_edge= <n></code> Range: {-1} ∪ [0, ∞[Unit: μm</p>
spacing	<p>Sets the uniform level-set grid spacing (the spacing is the same in the x-, y-, and z-direction, and is not spatially varying).</p> <p>Type: Number Default: none Range: (0, ∞) Unit: μm</p>
split_plots	<p>Specifies whether to write intermediate plots each to a different file.</p> <p>Type: Boolean Default: false</p>
structure	<p>Sets the name of the structure to be diffused.</p> <p>Type: Character Default: default_structure</p>
surface_accuracy	<p>Sets the maximum deviation between the decimated exposed surface and the original exposed surface.</p> <p>When set to -1, the used value is half of the structure-dependent spacing epsilon¹.</p> <p>It can be specified only if <code>surface_decimate=true</code>, or if you do not specify the <code>surface_decimate</code> parameter and specify <code>let surface_decimate=true</code>.</p> <p>Type: Number Default: Value set by <code>let decimate_accuracy=<n></code> Range: {-1} ∪ [0, ∞[Unit: μm</p>

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diffuse

Table 61 Parameters of diffuse command (Continued)

Parameter	Description
surface_decimate	<p>Specifies whether to decimate the exposed surface used as an operand of Boolean operations.</p> <p>Type: Boolean</p> <p>Default: Value set by <code>let surface_decimate=</code></p>
surface_min_angle	<p>Sets the smallest angle in the elements of the decimated exposed surface used as an operand of Boolean operations.</p> <p>It can be specified only if <code>surface_decimate=true</code>, or if you do not specify the <code>surface_decimate</code> parameter and specify <code>let surface_decimate=true</code>.</p> <p>Type: Number</p> <p>Default: Value set by <code>let surface_min_angle=<n></code></p> <p>Range: [0, 180]</p> <p>Unit: degree</p>
surface_min_dihedral_angle	<p>Sets the smallest dihedral angle between two elements, which share an edge, of the decimated exposed surface used as an operand of Boolean operations.</p> <p>It can be specified only if <code>surface_decimate=true</code>, or if you do not specify the <code>surface_decimate</code> parameter and specify <code>let surface_decimate=true</code>.</p> <p>Type: Number</p> <p>Default: Value set by <code>let surface_min_dihedral_angle=<n></code></p> <p>Range: [0, 180]</p> <p>Unit: degree</p>
surface_shortest_edge	<p>Sets the shortest edge of the decimated exposed surface used as an operand of Boolean operations. When set to -1, the used value is half of the structure dependent spacing <code>epsilon</code>¹.</p> <p>It can be specified only if <code>surface_decimate=true</code>, or if you do not specify the <code>surface_decimate</code> parameter and specify <code>let surface_decimate=true</code>.</p> <p>Type: Number</p> <p>Default: Value set by <code>let surface_shortest_angle= <n></code></p> <p>Range: {-1} ∪ [0, ∞[</p> <p>Unit: μm</p>

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diffuse

Table 61 Parameters of diffuse command (Continued)

Parameter	Description
temperature	Sets the spatially varying expression of the simulation temperature. The expression can contain the following variables: x, y, z, t, and field_names (fields). The variables field_names (fields) refer to those specified in the diffusion machine given by the machine parameter. Type: Character Default: 0 Range: (0, ∞) Unit: K
time	Sets the simulation time. Type: Number Default: none Unit: minute

1. The structure-dependent spacing epsilon is logged out when defining a structure using the define_structure command.

Examples

See Examples in [define_diffuse_machine on page 234](#).

etch

This command starts an etching simulation or a simultaneous etching and deposition simulation, as well as a deposition simulation based on a reaction model, and can be used in one of the following ways:

- Using a machine defined by `define_etch_machine`
- Geometrically etching a shape defined with the `define_shape` command
- Geometrically etching a mask defined with the `define_mask` command

Syntax

Etching simulation on the surface of the structure using a machine with `method=levelset`:

```
etch method=levelset spacing=<v> time=<n> \
[accuracy=<n>] [cfl=<n>] [comment=<c>] [decimate=<b>] \
[diffusion_flux_error_control_strategy=<c>] \
[diffusion_flux_integration_error=<n>] \
[engine=<c>] [exposed_only=<b>] \
[extraction=<c> (extraction_interval=<n> | \
extraction_times=<v> [extraction_times_unit=<c>]) \
[extraction_file_update_interval=<n>] \
[force_intermediate_extraction=<b>]] \
[file=<c>] [fill_material=<c>] [fill_region=<c>] \
[flat_orientation=<v>] \
[integration_error=<n> | integration_samples=<n>] \
[machine=<c>] [max_ion_reflections=<n>] \
([abs_min_deposition_thickness=<n>] | min_deposition_thickness=<n>) \
[merge=<b>] [min_angle=<n>] [min_dihedral_angle=<n>] \
[min_ion_reflection_probability=<n>] \
[pad_pressure_acceleration=<b>] [pad_pressure_accuracy=<n>] \
[pad_pressure_max_iterations=<n>] \
[(plot_interval=<n> [compute_first_plot=<b>]
[compute_last_plot=<b>] | \
plot_times=<v> [plot_times_unit=<c>]) \
[force_intermediate_plot=<b>] [num_flux_orders=<n>] \
[plot_file_update_interval=<n>] [plot_type=<l>] [split_plots=<b>]] \
[random_seed=<n>] [region=<c>] [region_query_accuracy=<c>] \
[remove_spurious_parts=<b>] [ridge_angle=<n>] \
[selective_deposition=<b> [selective_deposition_threshold=<n>]] \
[shortest_edge=<n>] [stop_plane=<n> | stop_point=<w>] \
[structure=<c>] [surface_accuracy=<n>] [surface_decimate=<c>] \
[surface_min_angle=<n>] [surface_min_dihedral_angle=<n>] \
[surface_ridge_angle=<n>] [surface_shortest_edge=<n>] \
[update_scheme=<c>] [variance_reduction=<c>] \
[vertical_orientation=<v>]
```

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etch

Note:

The `fill_material` and `fill_region` parameters are not available for simultaneous etching and deposition models.

Etching using a machine with `method=levelset` is not supported when the structure specified with the parameter `structure` is a PMC structure. To process such a structure, an explicit conversion of the structure is needed before calling the `etch` command (see [Integration With Other Sentaurus Topography 3D Functionality on page 580](#)).

Etching simulation on the surface of the structure using a machine with `method=pmc`:

```
etch method=pmc spacing=<v> time=<n> \
[averaging_interval=<n> | \
averaging_times=<v> [averaging_times_unit=<c>]] \
[averaging_runs=<n>] \
[comment=<c>] [compute_process_graph=<b>] [deposition_method=<c>] \
[electric_field_update_accuracy=<n>] \
[electric_field_update_interval=<n>] \
[electric_solver=<c>] \
[extraction=<c> (extraction_interval=<n> | \
extraction_times=<v> [extraction_times_unit=<c>])) \
[extraction_file_update_interval=<n>] \
[force_intermediate_extraction=<b>]] \
[file=<c>] [force_html_report=<b>] [force_intermediate_plot=<b>] \
[html_report=<b>] \
[html_report_interval=<n> | (html_report_times=<v> \
[html_report_times_unit=<c>])] [html_report_type=<c>] \
[machine=<c>] [max_number_edges_process_graph=<n>] \
[max_number_reflections=<n>] \
[noise_reduction=<n>] \
[num_trajectories=<n> | trajectory_starting_positions=<l>] \
[(plot_interval<n> [compute_first_plot=<b> compute_last_plot=<b>] | \
plot_times<v> [plot_times_unit=<c>]) \
[plot_type=<l> [force_intermediate_plot=<b>] \
[gc_samples_per_cell=<n>] \
[num_flux_orders=<n>] [plot_quality=<n>] \
[point_max=<v> point_min=<v>]]] \
[save_averaging_samples=<b> [averaging_sample_base_name=<c>]] \
[selective_deposition=<b>] [split_replacements=<l>] \
[sputtering_method=<c>] \
[stop_function=<c>] \
[stop_function_interval=<n> | \
(stop_function_times=<v> [stop_function_times_unit=<c>]))] \
[stop_material=<c> | stop_plane=<n> | stop_point=<w>] \
[structure=<c>] \
[tcl_equivalent_flux_variable=<c>] [top_gas_thickness=<n>]
```

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etch

Geometric etching using a shape:

On a boundary structure:

```
etch shape=<c> \
  [accuracy=<n>] [comment=<c>] [decimate=<b>] [fill_material=<c>] \
  [fill_region=<c>] [material=<c>] [min_angle=<n>] \
  [min_dihedral_angle=<n>] \
  [ridge_angle=<n>] [shortest_edge=<n>] [structure=<c>]
```

On a PMC structure:

```
etch shape=<c> \
  [comment=<c>] [fill_material=<c>] [material=<c>] [structure=<c>]
```

Geometric etching using a mask:

On a boundary structure:

```
etch mask=<c> thickness=<n> type=<c> \
  [accuracy=<n>] [comment=<c>] [decimate=<b>] [fill_material=<c>] \
  [fill_region=<c>] [min_angle=<n>] [min_dihedral_angle=<n>] \
  [ridge_angle=<n>] [shortest_edge=<n>] [structure=<c>]
```

On a PMC structure:

```
etch mask=<c> thickness=<n> type=<c> \
  [comment=<c>] [fill_material=<c>] [structure=<c>]
```

Similar to the `pattern` command, geometric etching using a mask conveniently combines several processing steps. It can be interpreted as a shortcut for the following process steps:

- Deposition of a negative or positive resist
- Exposure of the resist with a dark-field or a light-field reticle
- Development of the resist
- Geometric etching of the structure
- Stripping of the resist

Note:

Geometric etching using a mask is not supported for 2D structures.

Geometric etching using a shape or using a mask is not supported when the structure specified with the parameter `structure` is a PMC structure. To process such a structure, an explicit conversion of the structure is needed before calling the `etch` command (see [Integration With Other Sentaurus Topography 3D Functionality on page 580](#)).

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command

Parameter	Description
abs_min_deposition_thickness	<p>Sets the absolute minimum thickness a deposited layer must grow during a time step to be created or added.</p> <p>Type: Number</p> <p>Default: 0</p> <p>Range: [0, ∞[</p> <p>Unit: μm</p>
accuracy	<p>Sets the maximum deviation between the decimated surface of the boundary structure produced by Boolean operations and its original surface.</p> <p>When set to -1, the used value is half of the structure-dependent spacing epsilon¹.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none"> • The <code>structure</code> parameter denotes a boundary structure. • You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number</p> <p>Default: Value set by <code>let decimate_accuracy=<n></code></p> <p>Range: {-1} ∪ [0, ∞[</p> <p>Unit: μm</p>
averaging_interval	<p>Sets the time interval after which the different PMC runs are averaged. If the parameter is omitted, the value of the <code>time</code> parameter is used.</p> <p>Type: Number</p> <p>Default: none</p> <p>Range:]0, ∞[</p> <p>Unit: minute</p>
averaging_runs	<p>Sets the number of PMC runs to be averaged.</p> <p>Type: Number</p> <p>Default: 1</p> <p>Range: [1, ∞[</p>

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
averaging_sample_base_name	<p>Sets the base name of the file names used to save the results of individual averaging runs in PMC format. The default is the value of the <code>base_name</code> parameter of the <code>let</code> command.</p> <p>Note: This parameter can be set only when <code>save_averaging_samples=true</code>.</p> <p>Type: Character Default: <base_name></p>
averaging_times	<p>Sets the times after which the different PMC runs are averaged. The given vector must:</p> <ul style="list-style-type: none"> Contain only nonnegative values Be sorted in ascending order Contain no value larger than the value of parameter <code>time</code> <p>Type: Vector Default: none</p>
averaging_times_unit	<p>Sets the unit of the <code>averaging_times</code> values. Options are:</p> <ul style="list-style-type: none"> s (seconds) min (minutes) <p>Type: Character Default: min</p>
cfl	<p>Sets the Courant–Friedrichs–Lowy (CFL) number [16] for the integration of the surface evolution equation.</p> <p>Type: Number Default: 0.95 (when using a machine having <code>model=simple</code>) 0.5 (when using a machine having not having <code>model=simple</code>) Range:]0, 1]</p>
comment	<p>Sets a comment for this process step that is displayed or written to the log file.</p> <p>Type: Character Default: empty string</p>

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
compute_first_plot	When <code>plot_interval</code> is set, the parameter <code>compute_first_plot</code> specifies whether to produce an intermediate plot at <code>time=0</code> . Type: Boolean Default: true
compute_last_plot	When <code>plot_interval</code> is set, the parameter <code>compute_last_plot</code> specifies whether to produce an intermediate plot at the end of the simulation. Type: Boolean Default: true
compute_process_graph	Specifies whether to compute the process graph during a PMC simulation. Note: This parameter can be specified only if <code>noise_reduction=0</code> or if <code>noise_reduction</code> is not specified. Type: Boolean Default: false
decimate	Specifies whether to decimate the boundary structure produced by Boolean operations. It can be specified only if <code>structure</code> denotes a boundary structure. Type: Boolean Default: Value set by <code>let decimate=</code>
deposition_method	Sets the PMC deposition method. The methods differ with respect to the surface diffusion model, which affects the smoothness and the shape evolution of the deposited film. Options are: <ul style="list-style-type: none"> • generic • layer • layer_minimum • minimum • patch Type: Character Default: minimum

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
diffusion_flux_error_control_strategy	Sets the value of the parameter diffusion_flux_integration_error. Options are: <ul style="list-style-type: none">• absolute: Absolute error.• relative: Relative error Type: Character Default: relative
diffusion_flux_integration_error	Sets the requested flux error of the diffusing species. Type: Number Default: 0.05 Range: [0, 1]
electric_field_update_accuracy	When simulating charge-up, this parameter sets a threshold used to determine whether to recompute the electric field. If the change of the local charges accumulated in the structure is greater than the given accuracy, then the electric field is updated. This check is performed at regular time intervals, specified by electric_field_update_interval. Type: Number Default: 0 (always update the electric field) Range: [0, ∞)
electric_field_update_interval	When simulating charge-up, you must specify the time interval after which the electric field is updated. Type: Number Default: none Range: (0, ∞) Unit: minute
electric_solver	When simulating charge-up, you can optionally set the name of an electric field solver object defined in the command define_electric_solver (see define_electric_solver on page 239). If not specified, then default parameters are used for the electric field solver. Type: Character Default: none

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
engine	Sets the engine to use for flux computation. This parameter is available only for flux models. Options are: <ul style="list-style-type: none">• monte_carlo• radiosity Type: Character Default: radiosity
exposed_only	Specifies whether only exposed portions of the surface are etched when using the simple model. Type: Boolean Default: false
extraction	Sets the name of the group of extractions to run during this process step. Type: Character Default: none
extraction_file_update_interval	Sets the time interval after which intermediate extraction results are written to file. When set to 0, intermediate extraction results are written to file immediately after they are created. Note: This parameter can be set only when at least one intermediate extraction produces file output. Type: Number Default: 0 Range: [0, ∞[Unit: minute
extraction_interval	Sets the process time interval after which intermediate extractions must be executed. Type: Number Default: none Range:]0, ∞[Unit: minute

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
extraction_times	<p>Sets the times at which to perform intermediate extractions. The given vector must:</p> <ul style="list-style-type: none"> • Contain only nonnegative values • Be sorted in ascending order • Contain no value larger than the value of parameter time <p>If any of these conditions is not met, then an error is issued.</p> <p>Type: Vector Default: none</p>
extraction_times_unit	<p>Sets the unit of the extraction_times values. Options are:</p> <ul style="list-style-type: none"> • s (seconds) • min (minutes) <p>Type: Character Default: min</p>
file	<p>Sets the file into which intermediate surfaces and surface data should be saved. Used in conjunction with plot_interval only.</p> <p>In the file name, <base_name> denotes the value of the base_name parameter of the let command.</p> <p>Type: Character Default: <base_name>.tdr</p>
fill_material	<p>Sets the material to fill the etched volume. If this parameter is omitted, the etched volume is not filled.</p> <p>Type: Character Default: none</p>
fill_region	<p>Sets the name of the region filling the etched volume. The structure specified with the parameter structure must not contain regions with this name. If fill_region is omitted, the name of the region filling the etched volume is generated automatically. It can be specified only if structure denotes a boundary structure.</p> <p>Type: Character Default: none</p>

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
flat_orientation	Sets the Miller index of the direction perpendicular to the wafer flat (y-axis of the wafer coordinate system) for the newly created region for models that perform simultaneous etching and deposition. Type: Vector Default: {1 1 0}
force_html_report	Specifies whether to produce a report about the performed PMC simulation even if Sentaurus Topography 3D was started with the --no_html_report command-line option. Type: Boolean Default: false
force_intermediate_extraction	Specifies whether to compute intermediate extractions and, if applicable, write them to files even if Sentaurus Topography 3D was started with the command-line option --no_intermediate_extraction. Type: Boolean Default: false
force_intermediate_plot	Specifies whether to compute intermediate plots and write them to files even if Sentaurus Topography 3D was started with the --no_intermediate_plot command-line option. Type: Boolean Default: false
gc_samples_per_cell	Sets the number of samples to take along the x- and y-directions per grid cell. Type: Number Default: 1 Range: [1, 2147483647]
html_report	Specifies whether to produce a report (HTML file) about the performed PMC simulation. If neither html_report_interval nor html_report_times is specified, then the report is produced at the end of the simulation. Type: Boolean Default: true

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
html_report_interval	<p>Sets the process time interval after which HTML reports must be produced.</p> <p>Type: Number</p> <p>Default: none</p> <p>Range:]0, ∞[</p> <p>Unit: minute</p>
html_report_times	<p>Sets the times at which to create HTML reports. The given vector must:</p> <ul style="list-style-type: none"> Contain only nonnegative values Be sorted in ascending order Contain no value larger than the value of parameter time <p>If any of these conditions is not met, then an error is issued.</p> <p>Type: Vector</p> <p>Default: none</p>
html_report_times_unit	<p>Sets the unit of the html_report_times values.</p> <p>Options are:</p> <ul style="list-style-type: none"> min (minutes) s (seconds) <p>Type: Character</p> <p>Default: min</p>
html_report_type	<p>Sets the HTML report type to produce. Options are:</p> <ul style="list-style-type: none"> cumulative (reported statistics are collected starting from the beginning of the simulation) differential (reported statistics are collected starting from when the previous HTML report was produced) <p>Type: Character</p> <p>Default: cumulative</p>
integration_error	<p>Sets the maximum relative discretization error in the direct flux calculation.</p> <p>Type: Number</p> <p>Default: 0.05</p> <p>Range:]0, 1]</p>

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
integration_samples	<p>Sets the number of integration points in the numeric integration.</p> <p>The meaning of this parameter depends on the value of the <code>engine</code> parameter:</p> <ul style="list-style-type: none"> • When <code>engine=radiosity</code>, <code>integration_samples</code> describes the number of discretization points, per surface element, in the hemisphere where visibility is determined. • When <code>engine=monte_carlo</code>, <code>integration_samples</code> describes the number of particle paths, per surface element, used in the flux integration. <p>Note: This parameter is deprecated for <code>engine=radiosity</code>. Instead, use the <code>integration_error</code> parameter.</p> <p>Type: Number Default: 1000 (<code>engine=radiosity</code>), 700 (<code>engine=monte_carlo</code> and <code>variance_reduction= M-2016.12</code>), 350 (<code>engine=monte_carlo</code> and <code>variance_reduction= N-2017.09</code>) Range: [1, ∞[</p>
machine	<p>Sets the name of the machine that is used for the etch process.</p> <p>Type: Character Default: <code>default_machine</code></p>
mask	<p>Sets the name of the mask to be used for the etch process.</p> <p>Type: Character Default: none</p>
material	<p>Sets the material that can be etched. If omitted, all materials can be etched.</p> <p>Type: Character Default: none</p>

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
max_ion_reflections	Sets the maximum number of ion reflections to compute during flux integration. The specified value must be an integer. Only applicable when using RFM models. Type: Number Default: 1 Range: [1, ∞[
max_number_edges_process_graph	Sets the maximum number of edges of the process graph that can be visualized. Type: Number Default: 10000 Range: [1, 2147483647]
max_number_reflections	Sets the number of reflections a species can undergo before being discarded. Type: Number Default: 2000000 Range: [0, 2147483647]
merge	If true, then the deposited region merges with the already existing regions of the same material in the structure. Type: Boolean Default: false
method	Sets the simulation method to use. Options are: <ul style="list-style-type: none">• levelset• pmc Type: Character Default: levelset

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
min_angle	<p>Sets the smallest angle in the elements of the decimated surface of the boundary structure produced by Boolean operations.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none"> • The <code>structure</code> parameter denotes a boundary structure. • You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_min_angle=<n></code> Range: [0, 180] Unit: degree</p>
min_deposition_thickness	<p>Sets the minimum thickness a deposited layer must grow during a time step to be created or added as a fraction of the mean spacing.</p> <p>Type: Number Default: 0.01 Range: [0, 1]</p>
min_dihedral_angle	<p>Sets the smallest dihedral angle between two elements of the decimated surface of the boundary structure produced by Boolean operations that share an edge.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none"> • The <code>structure</code> parameter denotes a boundary structure. • You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_min_dihedral_angle=<n></code> Range: [0, 180] Unit: degree</p>
min_ion_reflection_probability	<p>Sets the threshold for the reflection probability below which multiple reflection is stopped.</p> <p>Type: Number Default: 0.001 Range: [0, 1]</p>

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
noise_reduction	<p>Specifies the amount of noise reduction.</p> <p>Note: This parameter can be specified only if the used model includes sputtering reactions.</p> <p>Type: Number Default: 0 Range: [0, 1]</p>
num_flux_orders	<p>Sets the number of flux orders to produce for each PMC intermediate surface plot. It can be specified only when <code>plot_type</code> contains the value <code>surface</code>.</p> <p>Type: Number Default: 1 Range: [1, 2147483647]</p>
num_trajectories	<p>When writing intermediate plots with <code>plot_type=trajectories</code>, this parameter sets the number of trajectories to be plotted.</p> <p>You can specify either <code>num_trajectories</code> or <code>trajectory_starting_positions</code>.</p> <p>Type: Number Default: 50 Range: [1, ∞)</p>
pad_pressure_acceleration	<p>Specifies whether to use an accelerated solver to evaluate the RFM function <code>pad_pressure()</code>.</p> <p>Note: You can set this parameter to false only when processing 2D structures.</p> <p>Type: Boolean Default: true</p>
pad_pressure_accuracy	<p>Sets the relative residual below which the solver stops when evaluating the RFM function <code>pad_pressure()</code>.</p> <p>Type: Number Default: 1e-3 Range: [0, ∞[</p>

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
pad_pressure_max_iterations	<p>Sets the maximum number of iterations that are allowed to evaluate the RFM function <code>pad_pressure()</code>.</p> <p>Type: Number</p> <p>Default: 100</p> <p>Range: [1, 2147483647]</p>
plot_file_update_interval	<p>Sets the time interval after which intermediate plots are written to file.</p> <p>When set to 0, intermediate plots are written to file immediately after they are created.</p> <p>Note: This parameter can be set only when <code>split_plots=false</code>.</p> <p>Type: Number</p> <p>Default: 0</p> <p>Range: [0, ∞[</p> <p>Unit: minute</p>
plot_interval	<p>Sets the process time interval after which intermediate exposed surfaces and surface data must be plotted.</p> <p>See TDR Dataset Names for Fluxes on page 429.</p> <p>Type: Number</p> <p>Default: none</p> <p>Range: [0, ∞[</p> <p>Unit: minute</p>
plot_quality	<p>Sets the quality of a PMC intermediate surface plot. The larger its value, the better the plot quality. It can be specified only when <code>plot_type=surface</code>.</p> <p>Type: Number</p> <p>Default: 1</p> <p>Range:]0, ∞[</p>

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
plot_times	<p>Sets the times at which to create intermediate plots. The given vector must:</p> <ul style="list-style-type: none">• Contain only nonnegative values• Be sorted in ascending order• Contain no value larger than the value of parameter time <p>If any of these conditions is not met, then an error is issued.</p> <p>Type: Vector Default: none</p>
plot_times_unit	<p>Sets the unit of the plot_times values. Options are:</p> <ul style="list-style-type: none">• s (seconds)• min (minutes) <p>Type: Character Default: min</p>
plot_type	<p>Sets the type of data to save at time intervals specified by plot_interval.</p> <p>When method=levelset, options are:</p> <ul style="list-style-type: none">• structure• surface <p>When method=pmc, options are:</p> <ul style="list-style-type: none">• charge_density• electric_field• electric_potential• gc• surface• vbe• volume_fractions <p>Type: List Default: surface</p>

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
point_max	<p>Sets the requested maximum corner of the bounding box of the grid containing the data. It can be set only when <code>plot_type=charge_density, electric_field, electric_potential, or volume_fractions</code>.</p> <p>The actual maximum corner of the bounding box of the grid containing the data is obtained by snapping the given <code>point_max</code> value to a grid point of the PMC structure (specified with the parameter <code>structure</code>).</p> <p>Type: Vector Default: automatic Unit: μm</p>
point_min	<p>Sets the requested minimum corner of the bounding box of the grid containing the data. It can be set only when <code>plot_type=charge_density, electric_field, electric_potential, or volume_fractions</code>.</p> <p>The actual minimum corner of the bounding box of the grid containing the data is obtained by snapping the given <code>point_min</code> value to a grid point of the PMC structure (specified with the parameter <code>structure</code>).</p> <p>Type: Vector Default: automatic Unit: μm</p>
random_seed	<p>Sets the seed of the pseudo-random number generator used by the Monte Carlo flux integrator.</p> <p>Note: This parameter can be specified only when <code>engine=monte_carlo</code>.</p> <p>Type: Number Default: 1 Range: [1, 2147483647]</p>
region	<p>Sets the name of the region that can be redeposited in advanced etching models. Not valid for etching models that do not create redeposition phenomena.</p> <p>Type: Character Default: none</p>

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
region_query_accuracy	<p>Sets the accuracy used to determine the regions and materials associated with each element of the exposed surface. Options are:</p> <ul style="list-style-type: none"> • resolution • subresolution <p>See Discretization Size and Accuracy on page 26.</p> <p>Type: Character Default: resolution</p>
remove_spurious_parts	<p>Specifies whether to remove spurious parts after running the process step.</p> <p>Type: Boolean Default: true</p>
ridge_angle	<p>Sets the angle used by the decimation algorithm to determine geometric features of the boundary structure produced by Boolean operations.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none"> • The <code>structure</code> parameter denotes a boundary structure. • You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_ridge_angle=<n></code> Range: [0, 180] Unit: degree</p>
save_averaging_samples	<p>Specifies whether to save the result of each averaging run in PMC format.</p> <p>Note: This parameter can be set only when the value of parameter <code>averaging_runs</code> is greater than 1.</p> <p>Type: Boolean Default: false</p>

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
selective_deposition	<p>Specifies whether to suppress the surface spreading of deposited material across material interfaces, thereby avoiding lateral creeping of the deposited film.</p> <p>Type: Boolean</p> <p>Default: false (for method=levelset) true (for method=pmc)</p>
selective_deposition_threshold	<p>Sets the threshold for the thickness of a layer below which the deposited material is considered to be an artifact. The specified value is relative to the mean discretization size.</p> <p>Type: Number</p> <p>Default: 1.0</p> <p>Range: [0.0, ∞[</p>
shape	<p>Sets the name of the shape that is used for the etch process.</p> <p>Type: Character</p> <p>Default: none</p>
shortest_edge	<p>Sets the shortest edge of the decimated surface of the boundary structure produced by Boolean operations. When set to -1, the used value is half of the structure-dependent spacing epsilon¹. This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none"> The structure parameter denotes a boundary structure. You specify decimate=true or, if you do not specify decimate, you did not specify let decimate=false. <p>Type: Number</p> <p>Default: Value set by let decimate_shortest_edge=<n></p> <p>Range: {-1} ∪ [0, ∞[</p> <p>Unit: μm</p>

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
spacing	<p>Sets the size of a grid cell for each direction. A vector with one component can be used to set the grid cell size to the same value for all dimensions. When <code>method=pmc</code>, this is the only supported option. Whereas, when <code>method=levelset</code>, nonuniform grid cell sizes are supported. When <code>method=levelset</code>, for 2D and 3D structures, a vector with two and three components, respectively, can be used to specify the grid cell size separately for each dimension. See Discretization Size and Accuracy on page 26.</p> <p>Type: Vector Default: none Unit: μm</p>
split_plots	<p>Specifies whether to write intermediate plots each to a different file.</p> <p>Type: Boolean Default: false</p>
split_replacements	<p>Specifies a list of material replacement maps defined in the command <code>define_material_replacement</code>. The list consists of the names of material replacement maps. The material is replaced by a list of species defined by the material replacement map before the PMC step begins.</p> <p>Note: This parameter can be used only with <code>method=pmc</code>.</p> <p>Type: List Default: none</p>
sputtering_method	<p>Sets the method to use when calculating from where to remove the material to be sputtered, with respect to the impact location of the incoming particle, which affects the smoothness and shape evolution of the structure. Options are:</p> <ul style="list-style-type: none"> • minimum • patch <p>Type: Character Default: minimum</p>

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
stop_function	<p>Sets the name of the Tcl procedure to invoke during a PMC simulation to determine whether to stop the simulation or to let it continue.</p> <p>The specified Tcl procedure must fulfill the following requirements:</p> <ul style="list-style-type: none">• It must have exactly one parameter (when invoking this Tcl procedure, Sentaurus Topography 3D sets this parameter to the current simulation time in minutes).• It must return a value on each execution path. The return value must be either 0 (or <code>false</code>) or 1 (or <code>true</code>). <p>The return value determines whether to stop the simulation. The return value 0 (or <code>false</code>) makes the simulation continue; the return value 1 (or <code>true</code>) makes the simulation stop.</p> <ul style="list-style-type: none">• Its body does not use Sentaurus Topography 3D commands other than <code>extract</code> and <code>save</code>. <p>If any of these requirements is not met, then an error message is issued when the specified Tcl procedure is invoked.</p> <p>Note:</p> <p>All structures defined in the current simulation are accessible to the <code>extract</code> and <code>save</code> commands within the specified Tcl procedure.</p> <p>The structure under processing is available as a PMC structure, independently of the initial structure type.</p> <p>Type: Character Default: none</p>
stop_function_interval	<p>Sets the process time interval after which the Tcl function specified by <code>stop_function</code> must be invoked.</p> <p>Type: Number Default: none Range:]0, ∞[</p>

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
stop_function_times	<p>Sets the times at which to invoke the Tcl function specified by <code>stop_function</code>. The given vector must:</p> <ul style="list-style-type: none">• Contain only nonnegative values• Be sorted in ascending order• Contain no value greater than the value of parameter <code>time</code> <p>If any of these conditions is not met, then an error message is issued.</p> <p>Type: Vector Default: none</p>
stop_function_times_unit	<p>Sets the unit of the <code>stop_function_times</code> values.</p> <p>Options are:</p> <ul style="list-style-type: none">• <code>min</code> (minutes)• <code>s</code> (seconds) <p>Type: Character Default: <code>min</code></p>
stop_material	<p>Sets the bulk material where etching stops etching when the surface reaches the specified material.</p> <p>When <code>method=pmc</code>, the <code>stop_material</code> parameter can stop etching when the specified material is used for the first time as a bulk material in a reaction.</p> <p>Type: Character Default: none</p>
stop_plane	<p>Sets the vertical coordinate of a horizontal plane below the exposed surface and not intersecting any void.</p> <p>When the exposed surface reaches or crosses this plane, time-stepping stops. See Stopping Time-Stepping on page 428.</p> <p>Type: Number Default: none Unit: μm</p>

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
stop_point	<p>Specifies a list of coordinates of points below the exposed surface and not inside any void. When the exposed surface reaches or crosses any of these points, the simulation stops. See Stopping Time-Stepping on page 428.</p> <p>Type: Vector list Default: none Unit: μm</p>
structure	<p>Sets the name of the structure to be etched.</p> <p>Type: Character Default: default_structure</p>
surface_accuracy	<p>Sets the maximum deviation between the decimated exposed surface and the original exposed surface. When set to -1, the used value is half of the structure-dependent spacing epsilon¹.</p> <p>It can be specified only if <code>surface_decimate=true</code>, or if you do not specify the <code>surface_decimate</code> parameter and specify <code>let surface_decimate=true</code>.</p> <p>Type: Number Default: Value set by <code>let decimate_accuracy=<n></code> Range: $\{-1\} \cup [0, \infty[$ Unit: μm</p>
surface_decimate	<p>Specifies whether to decimate the exposed surface used as an operand of Boolean operations.</p> <p>Type: Boolean Default: Value set by <code>let surface_decimate=</code></p>
surface_min_angle	<p>Sets the smallest angle in the elements of the decimated exposed surface used as an operand of Boolean operations.</p> <p>It can be specified only if <code>surface_decimate=true</code>, or if you do not specify the <code>surface_decimate</code> parameter and specify <code>let surface_decimate=true</code>.</p> <p>Type: Number Default: Value set by <code>let surface_min_angle=<n></code> Range: $[0, 180]$ Unit: degree</p>

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
surface_min_dihedral_angle	<p>Sets the smallest dihedral angle between two elements, which share an edge, of the decimated exposed surface used as an operand of Boolean operations.</p> <p>It can be specified only if <code>surface_decimate=true</code>, or if you do not specify the <code>surface_decimate</code> parameter and specify <code>let surface_decimate=true</code>.</p> <p>Type: Number Default: Value set by <code>let surface_min_dihedral_angle=<n></code> Range: [0, 180] Unit: degree</p>
surface_ridge_angle	<p>Sets the angle used by the decimation algorithm to determine geometric features of the exposed surface used as an operand of Boolean operations. It can be specified only if <code>surface_decimate=true</code>, or if you do not specify the <code>surface_decimate</code> parameter and specify <code>let surface_decimate=true</code>.</p> <p>Type: Number Default: Value set by <code>let surface_ridge_angle=<n></code> Range: [0, 180] Unit: degree</p>
surface_shortest_edge	<p>Sets the shortest edge of the decimated exposed surface used as an operand of Boolean operations. When set to -1, the used value is half of the structure dependent spacing <code>epsilon</code>¹.</p> <p>It can be specified only if <code>surface_decimate=true</code>, or if you do not specify the <code>surface_decimate</code> parameter and specify <code>let surface_decimate=true</code>.</p> <p>Type: Number Default: Value set by <code>let surface_shortest_angle=<n></code> Range: {-1} ∪ [0, ∞[Unit: μm</p>

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
tcl_equivalent_flux_variable	<p>Sets the name of the Tcl variable to which the equivalent fluxes will be written.</p> <p>When the <code>etch</code> command is executed, this Tcl variable will contain a list with an entry for each volumetric source species. Each entry is, in turn, a list of two elements containing the volumetric source species name and its equivalent flux.</p> <p>If you omit this parameter, then no Tcl output is produced.</p> <p>Type: Character Default: none</p>
thickness	<p>Sets the etch depth when etching with a mask, measured relative to the exposed surface of the structure.</p> <p>Type: Number Default: none Range: [0, ∞[Unit: μm</p>
time	<p>Sets the simulation time.</p> <p>Type: Number Default: none Unit: minute</p>
top_gas_thickness	<p>Sets the minimum thickness of the gas region added on top of the structure.</p> <p>Type: Number Default: 0 Range: [0, ∞[Unit: μm</p>

Chapter 6: Input Commands

etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
trajectory_starting_positions	<p>When writing intermediate plots with <code>plot_type=trajectories</code>, this parameter sets the starting positions of the trajectories on the xy plane above the structure. The starting positions must be given as a list of xy pairs: <code>{x1 y1 x2 y2 ...}</code>. You can specify either <code>num_trajectories</code> or <code>trajectory_starting_positions</code>.</p> <p>Type: List Default: none Unit: μm</p>
type	<p>Sets the type of the reticle and the resist. Options are:</p> <ul style="list-style-type: none">• <code>dark_negative</code>• <code>dark_positive</code>• <code>light_negative</code>• <code>light_positive</code> <p>Type: Character Default: none</p>
update_scheme	<p>Sets the update scheme for the time integration of the level-set function. Options are:</p> <ul style="list-style-type: none">• <code>lax_friedrichs</code>• <code>upwind</code> <p>Type: Character Default: <code>upwind</code></p>
variance_reduction	<p>Sets the algorithm to use for variance reduction by the Monte Carlo flux integrator. Options are:</p> <ul style="list-style-type: none">• <code>N-2017.09</code>• <code>M-2016.12</code> <p>Type: Character Default: <code>N-2017.09</code></p>

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etch

Table 62 Parameters of etch command (Continued)

Parameter	Description
vertical_orientation	Sets the Miller index of the direction perpendicular to the wafer surface (z-axis of the wafer coordinate system) for the newly created region for models that perform simultaneous etching and deposition. Type: Vector Default: {0 0 1}

1. *The structure-dependent spacing epsilon is logged out when defining a structure using the define_structure command.*

Note:

The Miller indices for a plane are usually written as (hkl), and the set of equivalent planes is written as {hkl}. A crystal direction is usually written as [hkl], and the set of equivalent directions is written as <hkl>. The value assigned to the parameters flat_orientation and vertical_orientation is a Tcl list of indices representing a crystal direction. The braces in the specified value are required to form a Tcl list and do not indicate a set of equivalent planes.

Limitations

The following limitations apply:

- When method=pmc, the grid spacing specified with the parameter spacing is ignored if the structure specified with the parameter structure stores the result of a previous simulation using the PMC method.
- When running a simulation with a machine using a reaction model that allows deposition, the vertical extent of the computational domain (see [Boundary Types on page 31](#)) must be large enough to contain the deposited material. The vertical extent of the computational domain can be increased by adding Gas to the initial structure using the fill command (see [fill on page 477](#)).
- For machines using RFM models with a rate formula involving the function pad_pressure(), 2D structures whose exposed surface cannot be described as a single-valued function of the x-coordinate are not supported.
- When using a machine with model=crystal, the following parameters are not supported:

```
abs_min_deposition_thickness, cfl, compute_first_plot,  
compute_last_plot, extraction_interval, extraction_times,  
extraction_times_unit, file, min_deposition_thickness, plot_interval,  
plot_times, plot_times_unit, plot_type, region_query_accuracy,  
stop_plane, stop_point, update_scheme
```

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etch

- When you start Sentaurus Topography 3D with the `--processes` command-line option with a value greater than 1 (see [Table 1 on page 18](#)), except when using `method=pmc`, the parameter structure must not denote a structure obtained from the `etch` command using `method=pmc averaging_runs=1`.
- When you start Sentaurus Topography 3D with the `--processes` command-line option with a value greater than 1 (see [Table 1 on page 18](#)) and use `method=pmc averaging_runs=1`:
 - The following parameters are not supported:
`extraction, plot_interval, plot_times, stop_material, stop_plane, stop_point`
 - The parameter `compute_process_graph=true` is not supported.
 - Machines using the parameter `damage` or volumetric source species are not supported.
 - Structures using periodic boundary conditions are not supported.

Examples

Etching process using an etch machine:

```
etch machine=etchmachine spacing={0.05 0.3 0.05} time=0.5
```

This command simulates an etching process on the structure, using the machine `etchmachine` with a grid spacing of $dx=0.05 \mu\text{m}$, $dy=0.3 \mu\text{m}$, $dz=0.05 \mu\text{m}$, and a simulation time of 0.5 minutes.

Note:

The resolution is adjusted internally to match the actual structure.

Etching process using a shape:

```
etch shape=shape_1 comment="etch shape"
```

This command etches the shape `shape_1` from the structure. The comment for this process step is displayed in the log file.

Etching process using a mask:

```
etch mask=mask_1 thickness=0.1 comment="etch mask"
```

This command uses the mask `mask_1` to etch $0.1 \mu\text{m}$, measured relative to the exposed surface of the structure. The comment for this process step is displayed in the log file.

Etching process with intermediate surface plotting:

```
etch machine=etchmachine spacing={0.1} time=0.5 \
    file=etch_surfaces.tdr plot_interval=0.1
```

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etch

This command etches using the machine `etchmachine`, with a grid spacing of $dx=dy=dz=0.1 \mu\text{m}$. Intermediate surfaces along with data such as surface velocities and fluxes are plotted into the file `etch_surfaces.tdr`. The surface of the first and last time steps of the simulation will always be plotted. During the simulation, whenever the simulation time surpasses an integral multiple of `plot_interval` (for example, 0.1, 0.2, 0.3, ...), a surface will be plotted to file. This feature is useful to check process parameters and model behavior.

Stopping Time-Stepping

This section discusses how to stop time-stepping.

Level Set Models

The `stop_plane` and `stop_point` parameters of the `etch` command are used in the same way as for the `deposit` command (see [Stopping Time-Stepping on page 389](#)).

The only differences are the constraints on the values specified with `stop_plane` and `stop_point`:

- When using `stop_plane`, the specified plane must intersect the computational domain. In addition, the specified plane must be below the initial exposed surface and must not intersect any voids.
- When using `stop_point`, the specified points must lie in the computational domain. In addition, the specified points must be below the exposed surface and must not lie inside any void.

PMC Models

For `method=pmc`, in addition to `stop_plane` and `stop_point`, the `stop_function` and `stop_material` parameters are available.

Example

```
proc my_stop_function { t_min } {
    set res [extract type=probe property=length axis=z \
        point={0.5 0.5 0}]
    if { $res < 0.5 } {
        return 1
    }
    return 0
}
...
etch spacing=0.02 time=1 method=pmc \
    stop_function_times={0 0.5 0.6 0.7 0.8 0.9 1} \
    stop_function=my_stop_function
```

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etch

In this example, the PMC simulation stops, and the `etch` command returns when the specified `stop_function`, called `my_stop_function`, returns 1.

The function `my_stop_function` returns 1 when the length of the material segment along the vertical line passing through point `{0.5 0.5 0}` becomes less than 0.5 µm. The command `extract` is used within the Tcl function to measure the length of the material segment along the specified line.

The function `my_stop_function` is invoked at simulation times 0 min., 0.5 min., 0.6 min., 0.7 min., 0.8 min., 0.9 min., and 1 min., as specified by the `stop_function_times` parameter.

TDR Dataset Names for Fluxes

For models that calculate ion or neutral fluxes, the values of the fluxes are written to TDR datasets when using the parameter `plot_interval`.

The name of a flux dataset starts with the name of the flux species. If the flux takes a yield function into account, it is followed by `yield`.

The type of flux is indicated by one of the following suffixes:

<code>direct</code>	The direct flux that arrives from the plasma at a surface element.
<code>reactive</code>	The incoming flux at a surface element that is available for reemission.
<code>reflected</code>	The direct flux that has been reflected away from a surface element.
<code>reflection</code>	The incoming flux at a surface element that has been reflected from other surface elements.
<code>total</code>	Sum of the reactive flux and the incoming indirect flux caused by the reactive flux.

Variance Reduction in PMC Simulations

PMC simulations use pseudo-random numbers to compute the evolution of the structure under the specified process conditions. When the sequence of pseudo-random numbers changes (for example, due to a different scheduling of the threads by the operating system), the results might also change, to an extent that depends on the model used and on the simulation parameters. This variability can be reduced by running the same simulation multiple times independently and by merging the different results.

You can control the number of PMC simulations to be run and merged together using the `averaging_runs` parameter. In addition, you can average the results at the end of the

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etch

simulation or after a certain amount of time, which can be specified by the averaging_interval parameter.

For example, the following command runs a PMC simulation of a 1 minute etching process 8 times and takes the average of the eight runs as the final result:

```
etch time=1 spacing=0.01 method=pmc averaging_runs=8
```

The following command splits the simulation time into five intervals, each of which is 0.2 minutes long:

```
etch time=1 spacing=0.01 method=pmc averaging_runs=8 \
averaging_interval=0.2
```

The evolution of the structure is simulated 8 times over each time interval, and the average of the obtained results is used as the initial structure for the simulation over the next interval.

When starting Sentaurus Topography 3D with a value of the `--processes` command-line option that is greater than 1, execution of the PMC-averaging runs is distributed over different processes using MPI. The processes run on the hosts specified with the `--mpi-file` command-line option (see [From the Command Line on page 17](#)).

Sentaurus Topography 3D tries to distribute the averaging runs evenly across the available processes, in a round-robin manner. When all PMC simulations are finished, the main process collects the results and averages them.

In addition, you can activate shared-memory parallelization of each PMC-averaging simulation (see [Basic Shared-Memory Parallelization on page 41](#) and [Advanced Shared-Memory Parallelization Options on page 42](#)).

Note:

For best performance, consider the following recommendations:

- Use a number of processes and hosts equal to the value of the `averaging_runs` parameter.
- The number of threads used on each node must not exceed the number of CPU cores available on the node. Use the `--threads` and `--max_threads` command-line options, or the `num_threads` parameter of the `let` command, to set the number of threads used by each process. Use the host file specified with the `--mpi-file` command-line option to specify the number of processes to run on each host. See [From the Command Line on page 17](#) and [let on page 501](#).

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extend_structure

extend_structure

This command extends a structure by mirroring it, or by copying and shifting it.

The initial structure and the extended structure merge automatically into one structure.

Note:

When you extend a structure by setting `type=shift`, the resulting structure might contain a path that connects the top gas with the bottom plane of the simulation domain, without passing through any other material. These types of structure are invalid for machine-based etching and deposition processes. There is no such problem with structures extended by mirroring.

Syntax

Extend a boundary structure:

```
extend_structure plane=<c> type=mirror \
[accuracy=<n>] [decimate=<b>] [min_angle=<n>] \
[min_dihedral_angle=<n>] [ridge_angle=<n>] \
[shortest_edge=<n>] [structure=<c>]

extend_structure plane=<c> type=shift \
[accuracy=<n>] [decimate=<b>] [min_angle=<n>] \
[min_dihedral_angle=<n>] [ridge_angle=<n>] \
[shortest_edge=<n>] [structure=<c>] [times=<n>]
```

Extend a PMC structure:

```
extend_structure plane=<c> type=mirror [structure=<c>]

extend_structure plane=<c> type=shift [structure=<c>] [time=1]
```

Note:

When you start Sentaurus Topography 3D with the `--processes` command-line option with a value greater than 1 (see [Table 1 on page 18](#)), the parameter `structure` must not denote a structure obtained from the `etch` command using `method=pmc averaging_runs=1`.

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extend_structure

Table 63 Parameters of *extend_structure* command

Parameter	Description
accuracy	<p>Sets the maximum deviation between the decimated surface of the boundary structure produced by Boolean operations and its original surface.</p> <p>When set to -1, the used value is half of the structure-dependent spacing epsilon¹.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none">• The <code>structure</code> parameter denotes a boundary structure.• You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_accuracy=<n></code> Range: $\{-1\} \cup [0, \infty[$ Unit: μm</p>
decimate	<p>Specifies whether to decimate the boundary structure produced by Boolean operations. It can be specified only if <code>structure</code> denotes a boundary structure.</p> <p>Type: Boolean Default: Value set by <code>let decimate=</code></p>
min_angle	<p>Sets the smallest angle in the elements of the decimated surface of the boundary structure produced by Boolean operations.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none">• The <code>structure</code> parameter denotes a boundary structure.• You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_min_angle=<n></code> Range: $[0, 180]$ Unit: degree</p>

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extend_structure

Table 63 Parameters of *extend_structure* command (Continued)

Parameter	Description
min_dihedral_angle	<p>Sets the smallest dihedral angle between two elements of the decimated surface of the boundary structure produced by Boolean operations that share an edge.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none">• The <code>structure</code> parameter denotes a boundary structure.• You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_min_dihedral_angle=<n></code> Range: [0, 180] Unit: degree</p>
plane	<p>Sets the side where the initial structure is extended (see Figure 29 on page 435). Options are:</p> <ul style="list-style-type: none">• back• front• left• right <p>Note: The values <code>back</code> and <code>front</code> apply only to 3D structures.</p> <p>Type: Character Default: none</p>
ridge_angle	<p>Sets the angle used by the decimation algorithm to determine geometric features of the boundary structure produced by Boolean operations.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none">• The <code>structure</code> parameter denotes a boundary structure.• You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_ridge_angle=<n></code> Range: [0, 180] Unit: degree</p>

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`extend_structure`

Table 63 Parameters of `extend_structure` command (Continued)

Parameter	Description
<code>shortest_edge</code>	<p>Sets the shortest edge of the decimated surface of the boundary structure produced by Boolean operations.</p> <p>When set to <code>-1</code>, the used value is half of the structure-dependent spacing <code>epsilon</code>¹.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none"> • The <code>structure</code> parameter denotes a boundary structure. • You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_shortest_edge=<n></code> Range: $\{-1\} \cup [0, \infty[$ Unit: μm</p>
<code>structure</code>	<p>Sets the name of the structure that is extended.</p> <p>Note: This parameter cannot specify a PMC structure. To process such a structure, an explicit conversion of the structure is needed before calling the <code>extend_structure</code> command (see Integration With Other Sentaurus Topography 3D Functionality on page 580).</p> <p>Type: Character Default: <code>default_structure</code></p>
<code>times</code>	<p>Sets the number of times the initial structure is copied and shifted.</p> <p>Type: Number Default: 1 Range: $[1, \infty[$</p>
<code>type</code>	<p>Sets the operation used to extend the initial structure. Options are:</p> <ul style="list-style-type: none"> • <code>mirror</code>: Mirror initial structure. • <code>shift</code>: Copy and shift initial structure. <p>Type: Character Default: <code>none</code></p>

1. The structure-dependent spacing `epsilon` is logged out when defining a structure using the `define_structure` command.

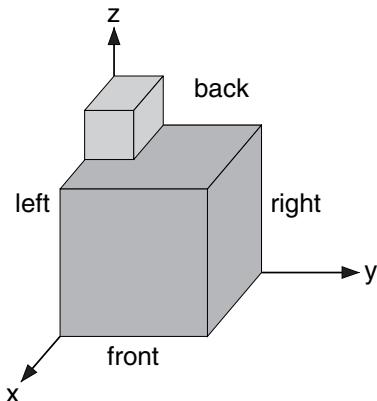
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extend_structure

Examples

[Figure 29](#) shows the initial structure used for these examples.

Figure 29 Initial structure and different values of the plane parameter

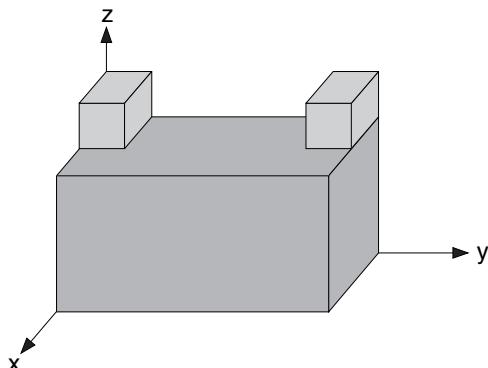


Extend the initial structure by mirroring at the xz plane at the maximum y -coordinate of the simulation domain:

```
extend_structure type=mirror plane=right
```

[Figure 30](#) shows the result of this command to the structure in [Figure 29](#).

Figure 30 Extending structure by mirroring



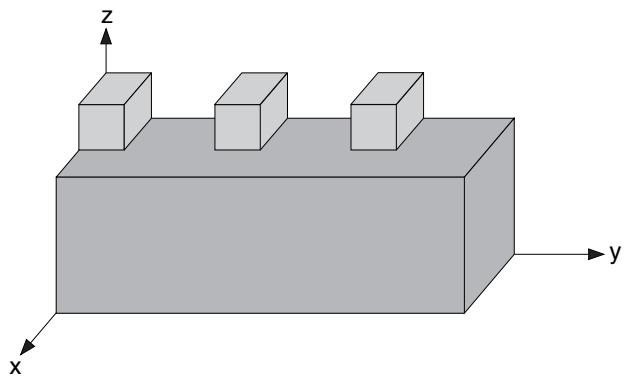
Extend the default structure by copying the default structure and shifting the copy to the xz plane at the maximum y -coordinate of the simulation domain. Then, a second copy is shifted to the maximum y -coordinate of the intermediate structure created by adding the first copy (see [Figure 31](#)):

```
extend_structure type=shift plane=right times=2
```

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extend_structure

Figure 31 Extending structure by copying and shifting twice



extract

This command extracts different properties of a structure and can be used more than once in the same command file.

The first time that you use the `extract` command with `type=1d_cut`, `type=2d_cut`, `type=interface`, `type=probe`, or `type=slice`, an extract file is created with the name specified with the parameter `file`. In subsequent uses of the command with the same value of the parameter `file`, the results are added to the previously computed and saved extractions. Each extraction has a name that is provided by the parameter `name`.

Note:

The `extract` command can extract properties from a structure only before or after a processing step. To extract properties during processing, see [define_extraction on page 252](#).

You can extract the following:

- [1D or 2D Cuts](#)
- [Properties of Exposed Surfaces](#)
- [Interface Area](#)
- [Areas and Volumes of Regions and Parts](#)
- [Region Names and Materials](#)
- [Region and Part Names](#)
- [Interface Position](#)
- [Intersections With a Line](#)
- [Intersections With a Plane](#)
- [Shortest Distance](#)
- [Shape Analysis](#)
- [Cylindrical Hole Profile](#)
- [Bounding Box of Materials and Regions](#)
- [Vertical Coordinates of the Top and Bottom of the Bounding Box of Materials and Regions](#)
- [Dimension of Structure](#)
- [Damage Integral](#)

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extract

- Surface Coverage
- Structure Spacing
- Structure Type

Specifying Extraction Lines, Planes, and Pairs

For some extractions, an extraction line, an extraction plane, or extraction pairs of materials or regions must be specified.

An extraction line can be specified in these different ways:

- Axis-aligned direction and one point:

```
axis=<c> point=<v>
```

- Arbitrary direction and one point:

```
direction=<v> point=<v>
```

- Two points:

```
point1=<v> point2=<v>
```

An extraction plane can be specified in these different ways:

- Axis-orthogonal plane at axis position:

```
axis=<c> position=<n>
```

- Arbitrary plane-normal direction and one point:

```
normal=<v> point=<v>
```

- Generic plane defined by three points:

```
point1=<v> point2=<v> point3=<v>
```

An extraction pair can be specified using pairs of identifiers:

- For two different materials:

```
material1=<c> material2=<c>
```

- For two different regions:

```
region1=<c> region2=<c>
```

- For two different parts:

```
region_part1=<l> region_part2=<l>
```

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extract

The names of regions can be extracted with `type=region_names` (see [Region Names and Materials on page 443](#)). Lists of region and part names can be extracted with `type=region_parts` (see [Region and Part Names on page 444](#)).

In the following syntax descriptions, the specifications for an extraction line, an extraction plane, and pairs of material or region are represented by `<extraction_line>`, `<extraction_plane>`, and `<extraction_pair>`, respectively.

Extraction Types

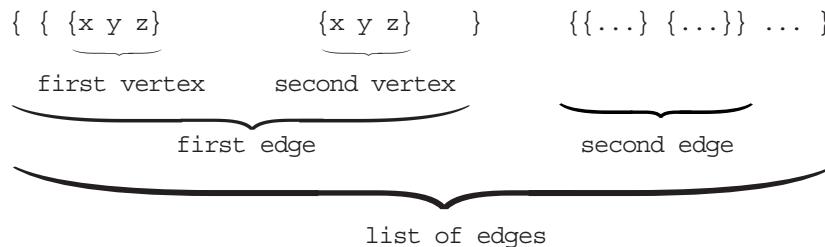
The extraction type is set with the parameter `type`.

1D or 2D Cuts

A `1d_cut` intersects the closed surface of a PMC structure or a boundary structure (defined in [Boundary Types on page 31](#)) with a line (the parameter `structure` must denote a boundary structure):

```
extract type=1d_cut <extraction_line> [file=<c>] [name=<c>] \
[silent=<b>] [structure=<c>]
```

The data returned by `type=1d_cut` is a list of edges represented in Tcl with the following format:



where:

- A vertex is a list of two or three floating-point numbers, depending on the dimension of the structure.
- An edge is a list of exactly two vertices.
- A 1D cut is a list of edges.

A `2d_cut` intersects the closed surface of a boundary structure with a plane (the parameter `structure` must denote a boundary structure):

```
extract type=2d_cut <extraction_plane> [file=<c>] [name=<c>] \
[silent=<b>] [structure=<c>]
```

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extract

Example: 1d_cut

```
extract axis=x point={-0.5 0.5 1.3} type=1d_cut
```

A line passing through the point (-0.5 0.5 1.3) and with a direction parallel to the x-axis is created and intersected with the closed surface. All the intersection points are written into a TDR file.

Extract the third coordinate of the second vertex of the second edge of a 1D cut:

```
set 1dcut = [extract axis=z point={0.5 0.5 0} type=1d_cut]
set edge1 [lindex $1dcut 1]
set vertex1 [lindex $edge1 1]
set coord2 [lindex $vertex1 2]
```

Example: 2d_cut

```
extract axis=z position=0.5 type=2d_cut
```

A plane with normal parallel to the z-axis and intersecting it at $z = 0.5$ is created and intersected with the closed surface. The intersection points are saved in a TDR boundary file. Every intersection between the plane and the closed surface has a name that is provided by the parameter `name`.

Note:

If not specified explicitly by setting the parameter `file`, 1D and 2D extractions are saved in the same TDR file.

Properties of Exposed Surfaces

To extract the bounding box of the exposed surface of a PMC structure or a boundary structure, use the command:

```
extract type=bounding_box_exposed [name=<c>] [silent=<b>] \
[structure=<c>]
```

It returns a list of the minimum and maximum vertices of the bounding box of the exposed surface.

To extract the minimum vertical coordinate of the exposed surface of a PMC structure or a boundary structure, use the command:

```
extract type=bottom_exposed [name=<c>] [silent=<b>] [structure=<c>]
```

To extract the maximum vertical coordinate of the exposed surface of a PMC structure or a boundary structure, use the command:

```
extract type=top_exposed [name=<c>] [silent=<b>] [structure=<c>]
```

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Example: bottom_exposed

```
extract type=bottom_exposed
```

This command extracts and outputs the minimum vertical coordinate of the bounding box of the exposed surface.

Example: bounding_box_exposed

```
extract type=bounding_box_exposed
```

This command extracts and outputs a list containing the minimum and maximum vertices of the bounding box of the exposed surface.

Example: top_exposed

```
extract type=top_exposed
```

This command extracts and outputs the maximum vertical coordinate of the bounding box of the exposed surface.

Interface Area

To extract the area of the interface between two regions of a boundary structure (the parameter `structure` must denote a boundary structure), use the command:

```
extract region_1=<c> region_2=<c> type=interface_area \
[name=<c>] [silent=<b>] [structure=<c>]
```

It returns the total area of the interface between the two specified regions.

Example: interface_area

```
extract type=interface_area region_1=substrate \
region_2=source_contact
```

This command extracts the area formed by the interface between the regions named `substrate` and `source_contact`.

The following commands show how to extract the interface area and assign it to a Tcl variable. Here, the output generated by the `extract` command is suppressed by setting `silent=true`:

```
set contact_area [extract type=interface_area region_1=substrate \
region_2=source_contact silent=true]
puts "The source contact area is $contact_area"
```

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Areas and Volumes of Regions and Parts

To extract geometric properties:

- Extraction of the surface area of a region of a boundary structure (the parameter structure must denote a boundary structure):

```
extract region=<c> type=area [name=<c>] [silent=<b>] \
[structure=<c>]
```

Returns the total surface area of the specified region.

- Extraction of the surface areas of the parts of a region of a boundary structure (the parameter structure must denote a boundary structure):

```
extract region=<c> type=part_area [name=<c>] [silent=<b>] \
[structure=<c>]
```

Returns the surface areas of all disconnected parts of the specified region as a Tcl list.

- Extraction of the volumes of the parts of a region of a boundary structure (the parameter structure must denote a boundary structure):

```
extract region=<c> type=part_volume [name=<c>] [silent=<b>] \
[structure=<c>]
```

Returns the volumes of all disconnected parts of the specified region as a Tcl list.

- Extraction of the volume of a region of a boundary structure (the parameter structure must denote a boundary structure):

```
extract region=<c> type=volume [name=<c>] [silent=<b>] \
[structure=<c>]
```

Returns the total volume of the specified region.

Example: area

```
extract type=area region=insulation
```

This command extracts the surface area of the region named insulation.

Example: part_area

```
extract type=part_area region=insulation
```

This command extracts the surface area of the individual parts of the region named insulation and creates the output separately.

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Example: part_volume

```
extract type=part_volume region=insulation
```

This command extracts the volume of the individual parts of the region named `insulation` and creates the output separately.

Example: volume

```
extract type=volume region=bulk
```

This command extracts and outputs the volume of the `bulk` region of the processed structure.

Region Names and Materials

To extract region names and materials:

- Extraction of the material names of a boundary structure (the parameter `structure` must denote a boundary structure):

```
extract type=material_names [exposed_only=<b>] [name=<c>] \
[silent=<b>] [structure=<c>]
```

Returns the names of the materials of a structure as a Tcl list.

- Extraction of the material names of a PMC structure (the parameter `structure` must denote a PMC structure):

```
extract type=material_names exposed_only=false [name=<c>] \
[silent=<b>] [structure=<c>]
```

Returns the names of the materials of a structure as a Tcl list.

- Extraction of region materials of a boundary structure (the parameter `structure` must denote a boundary structure):

```
extract region=<c> type=material_name [exposed_only=<b>] \
[name=<c>] [silent=<b>] [structure=<c>]
```

Returns the name of the material of the specified region.

- Extraction of region names of a boundary structure (the parameter `structure` must denote a boundary structure):

```
extract type=region_names [exposed_only=<b>] [name=<c>] \
[silent=<b>] [structure=<c>]
```

Returns the names of the regions of a structure as a Tcl list.

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Example: material_name

```
extract type=material_name region=insulation
```

This command extracts and outputs the name of the material of the insulation region.

Example: region_names

```
extract type=region_names
```

This command extracts and outputs the name of each region of the processed structure.

Region and Part Names

To extract the names of regions and the names of their parts:

- Extraction of all region and part names of a boundary structure (the parameter structure must denote a boundary structure):

```
extract type=region_parts [exposed_only=<b>] [name=<c>] \  
[silent=<b>] [structure=<c>]
```

Returns a list of pairs. The first element of each pair is the name of a region of the structure and the second element is a list of the names of the parts contained in that region.

- Extraction of part names of a region of a boundary structure (the parameter structure must denote a boundary structure):

```
extract region=<c> type=region_parts [exposed_only=<b>] \  
[name=<c>] [silent=<b>] [structure=<c>]
```

Returns a list containing the names of the parts in the given region.

Example: region_parts

```
extract type=region_parts
```

This command extracts and outputs the name of each part of each region of the processed structure.

The parts of a specific region can be extracted by specifying the region parameter:

```
extract type=region_parts region=mask
```

The name of each part of the region named mask is extracted and output separately.

Interface Position

To locate an interface between two different materials, or two different regions, or two different parts along a line in a structure, as well as to extract a vertex for the interface that

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the line passes through or a segment of the interface that the line is tangent to, use the command:

```
extract type=interface <extraction_line> <extraction_pair> \
[name=<c>] [output=<c>] [silent=<b>] [structure=<c>]
```

If you specify the `material1` and `material2` parameters, the special name `Gas` can be used to represent not only explicitly available gaseous regions, but also the empty space at the exposed surface. The parameters `material1` and `material2` are supported when the `structure` parameter denotes a boundary structure and when it denotes a PMC structure.

If you want to find interfaces between two specific but different regions of a boundary structure, use the `region1` and `region2` parameters. In this case, the `structure` parameter denotes a boundary structure.

To find the interfaces between two specific but different parts of a boundary structure, use the `region_part1` and `region_part2` parameters. In this case, the `structure` parameter denotes a boundary structure.

You can use the `output` parameter to filter the computed interface positions. It can have the following values:

- `output=all`: Along the input line, returns all interfaces in the output format described below. This is the default.
- `output=first`: Returns only the first interface.
- `output=inside`: Returns only the vertices or segments that are fully contained within or exactly on the `point1` to `point2` input segment. Only available if the `extract` command is specified with `point1` and `point2`.
- `output=last`: Returns only the last interface.
- `output=outside`: Returns only the vertices or segments that do not overlap the `point1` to `point2` input segment. Only available if the `extract` command is specified with `point1` and `point2`.

The data returned by `type=interface` is structured as follows:

```
{ {x y z} {x y z} {x y z x y z} ... }
```

Each element of this list represents either a vertex or a segment.

The exposed surface is treated specially with `type=interface`. An interface is returned for the exposed surface even if the input structure does not contain a gas region that touches the exposed surface. The material name `Gas` can always be used for one of the two parameters `material1` or `material2`, irrespective of whether the structure actually contains a gas region touching the exposed surface. On the other hand, specifying an interface using either `region1` and `region2`, or `region_part1` and `region_part2`, with an assumed gas region is not allowed.

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Example: interface

```
extract type=interface material1=Silicon material2=Oxide \
    point={0.5 0.5 0} direction={0 0 1}
```

This command extracts and outputs the interfaces between silicon and oxide in the processed structure along the specified line.

Intersections With a Line

Specifying `type=probe` intersects a structure with a line and returns a segment for each part of a region that the line passes through as well as a property associated with that segment, namely, the material name, or the region and part name:

```
extract type=probe <extraction_line> \
    (materials=<l> | [probe_empty_space=<b>]) \
    [name=<c>] [output=<c>] [property=<c>] [silent=<b>] [structure=<c>]
```

The `property` parameter specifies the data to be associated with each extracted segment in the returned value. This data refers to the part of a region where a segment comes from:

- `property=length`: The total length of the segments lying on the extraction line that go through the specified materials or through empty space. This property can be specified both when the `structure` parameter denotes a boundary structure and when it denotes a PMC structure.

If `probe_empty_space=false`, the total length of the segments lying on the extraction line that go through any material except `Gas` or empty space is returned.

If `probe_empty_space=true`, the total length of the segments lying on the extraction line that go through the material `Gas` or empty space is returned.

If the parameter `materials` is specified, the total length of the segments lying on the extraction line that go through the specified materials is returned.

- `property=material`: The material name of the underlying part of a region. This is the default and can be specified both when the `structure` parameter denotes a boundary structure and when it denotes a PMC structure.
- `property=region`: The region name of the underlying part. This property can be specified only when the `structure` parameter denotes a boundary structure.
- `property=region_part`: A list of two elements. The first element is the region name of the underlying part, and the second element is the name of the underlying part itself. The name of the underlying part is always a number. This property can be specified only when the `structure` parameter denotes a boundary structure.

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The `output` parameter can have the following values:

- `output=all`: Along the input line, returns all segments within regions in the output format described below. This is the default.
- `output=first`: Returns only the first entry.
- `output=inside`: Returns only the segments that are fully contained within or exactly on the `point1` to `point2` input segment. Only available if the `extract` command is specified with `point1` and `point2`.
- `output=last`: Returns only the last entry.
- `output=outside`: Returns only the segments that do not overlap the `point1` to `point2` input segment. Only available if the `extract` command is specified with `point1` and `point2`.

For `property=length`, the data returned by `type=probe` is a number that represents the sum of the length of the segments that lie in the specified materials or in empty space.

For `property=material`, `property=region`, and `property=region_part`, the data returned by `type=probe` is structured as follows:

```
{}{{x y z} {x y z} property} {}{{x y z} {x y z} property} ...}
```

The returned `property` is enclosed in double quotation marks if it contains spaces.

Example: probe

```
extract type=probe point1={0 0 0} point2={0 0 1} property=material
```

The processed structure is intersected with a line passing through the points of the coordinates `{0 0 0}` and `{0 0 1}`.

Intersections With a Plane

Specifying `type=slice` intersects a 3D boundary or PMC structure with a plane. The obtained 2D cut represents a 2D boundary that contains information about materials. The 2D boundary is saved into a TDR file:

```
extract type=slice <extraction_plane> [file=<c>] [name=<c>] \
[silent=<b>] [structure=<c>]
```

The obtained 2D cut is saved into a TDR file specified using the `file` parameter. The `structure` parameter must denote either a 3D boundary or PMC structure.

The saved structure can be used as input for a 2D simulation if the exposed surface of the structure (excluding voids) does not touch the bottom of the simulation domain (see [Boundary Types on page 31](#)). In other words, if you imagine pouring a liquid onto the

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structure, and the liquid does not reach the bottom of the rectangular domain, the structure is valid input for a simulation.

Example: slice

```
extract type=slice point={0 0 0} normal={0 1 0} file=slice.tdr
```

The processed structure is intersected with a plane having its normal direction parallel to the y-axis and passing through the point of the coordinates {0 0 0}. The 2D extracted boundary is saved in the TDR file named slice.tdr.

Shortest Distance

To extract the shortest distance between two different materials, or two different regions, or two different parts in a boundary structure (the `structure` parameter must denote a boundary structure), use the command:

```
extract type=shortest_distance <extraction_pair> \
[name=<c>] [silent=<b>] [structure=<c>]
```

The `material1` and `material2` parameters specify two different materials between which the shortest distance is sought.

The `region1` and `region2` parameters specify two different regions between which the shortest distance is sought. These two regions do not have to contain two different materials as in the case of the `material1` and `material2` parameters. All available parts of the two regions are considered in the search.

You can use `type=region_names` to extract a list of region names in a structure.

To find the shortest distance between two specific but different parts, use the `region_part1` and `region_part2` parameters.

You can use `type=region_parts` to extract a list of region and part names of a structure.

The data returned by `type=shortest_distance` is a list with the following two elements (an empty list is returned if one of the specified materials, regions, or parts does not exist in the structure, and a warning is issued):

```
{shortest_distance, segments}
```

The first element, `shortest_distance`, is the shortest distance measured in μm . The second element, `segments`, indicates where the shortest distance occurs. Since the shortest distance can occur at more than one location, `segments` is a list in the following format:

```
{segment1, ...} = { {vertex1, vertex2}, ... } = { { {x, y, z},  
{x, y, z} }, ... }
```

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The list contains only one segment if the shortest distance occurs uniquely at one specific location in the structure. When the shortest distance occurs at several locations, the number of segments depends on the discretization of the structure.

Example: `shortest_distance`

```
extract type=shortest_distance region_part1={mask 0} \
        region_part2={mask 1}
```

This command computes and returns the shortest distance between the parts named 0 and 1 of the `mask` region along with the segments where the shortest distance occurs. The command returns a list whose first element is the requested shortest distance.

Example of the extraction of the shortest distance from the returned value:

```
set res [extract type=shortest_distance region_part1={mask 0} \
                  region_part2={mask 1}]

set shortest_distance [lindex $res 0]
```

Shape Analysis

When you specify `type=shape_analysis`, the shape of a structure is analyzed and compared to the given reference shape (set by `reference_shape`). The `structure` parameter must denote a structure resulting from a level set or PMC simulation, and you must define a suitable domain containing the entire substructure to be analyzed.

For `reference_shape=cylinder_hole`, the syntax would be:

```
extract type=shape_analysis reference_shape=cylinder_hole \
        max_radius=<n> point1=<v> point2=<v> \
        [bottom_shift=<n>] [csv_file=<c>] [doe_parameters=<l>] \
        [extract_surface=<b>] [interface=<l>] [name=<c>] [output_type=<c>] \
        [smoothing_order=<n>] [structure=<c>] \
        [tdr_file=<c>] [top_shift=<n>] [vertical_spacing=<n>] [z_planes=<l>]
```

For `reference_shape=trench`, the syntax would be:

```
extract type=shape_analysis reference_shape=trench \
        max_depth=<n> max_width=<n> point1=<v> point2=<v> \
        [bottom_shift=<n>] [csv_file=<c>] [doe_parameters=<l>] \
        [extract_surface=<b>] [interface=<l>] [name=<c>] [output_type=<c>] \
        [smoothing_order=<n>] [structure=<c>] \
        [tdr_file=<c>] [top_shift=<n>] [vertical_spacing=<n>] [z_planes=<l>]
```

Different reference shapes are available:

- Set `reference_shape=cylinder_hole` to analyze a cylindrical hole structure.

You must specify a suitable cylindrical extraction window (a bounding box) around the structure of interest. The cylindrical bounding box is specified by two points (`point1` and

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`point2`) that define the bottom and top of the vertical cylinder axis, and by the radius (`max_radius`) of the cylinder (see [Figure 32 \(left\)](#)).

Note:

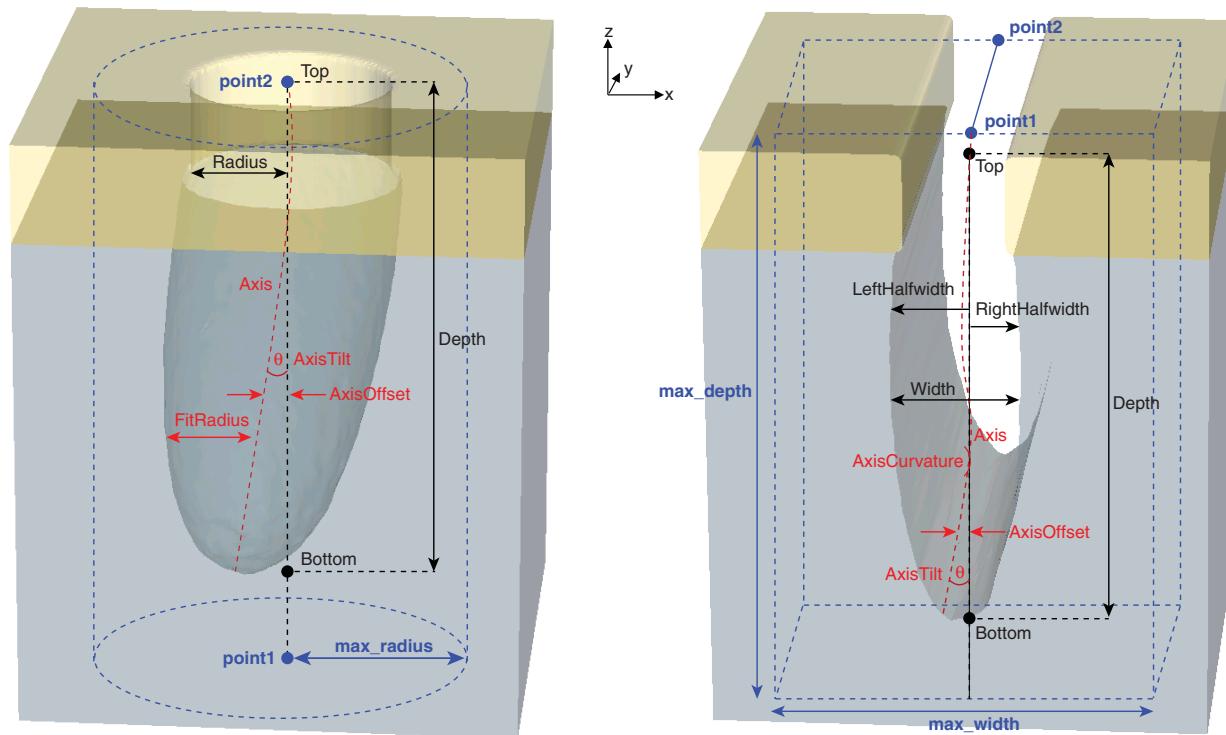
Only vertically aligned cylindrical bounding boxes are supported, that is, the x- and y-coordinates of `point1` and `point2` must coincide.

- Set `reference_shape=trench` to analyze a trench structure.

You must specify a suitable cuboid bounding box around the structure of interest. The orientation of the trench in the xy plane is specified by two points (`point1` and `point2`) that define the upper center line of the trench (see [Figure 32 \(right\)](#)). In addition, `point1` and `point2` must lie in the same xy plane (that is, their z-coordinates must coincide), but they can be arbitrarily oriented in the xy plane.

At the same time, `point1` and `point2` define the top and the orientation of the bounding box, which can have an arbitrary orientation in the xy plane, but must be vertically aligned with the z-axis. After you set `point1` and `point2`, set the width and depth of the bounding box by using the `max_width` and `max_depth` parameters.

Figure 32 Definition of extraction window for shape analysis when (left) reference_shape=cylinder_hole and (right) reference_shape=trench



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Data can be output in different ways:

- *Scalar data*, such as the hole depth, average tilt angle, bottom radius, top radius, and average hole radius, is returned as *design-of-experiments (DOE) parameters* to Sentaurus Workbench. You activate this feature by setting `output_type=doe`.

Optionally, you can specify the DOE parameters of interest using the parameter `doe_parameters={parameter1 parameter2 ...}`. If multiple extractions are executed, the name of the extractor (specified by parameter `name`) is prepended to the DOE name to distinguish different extractions. [Table 64 on page 453](#) lists the available DOE parameters for different values of `reference_shape`.

- *One-dimensional datasets*, such as the hole radius as a function of the z-axis, are written to a TDR file if `output_type=tdr` is set. By default, the file name is the base name of the command file with the suffix `_extract.tdr`. Alternatively, you can specify a file name with the parameter `tdr_file`. The resulting file can be visualized in Sentaurus Visual. [Table 65 on page 458](#) lists the available datasets for different values of `reference_shape`.

You can store datasets in a comma-separated value (CSV) format by setting `output_type=csv` with the same naming convention as for TDR files, but with the suffix `_extract.csv`. A different file name can be specified with the parameter `csv_file`.

- *Surface points*: If you set `extract_surface=true`, then you can extract the surface points of a hole or trench in the xy plane at different heights z, specified by a list of z-coordinates in parameter `z_planes` (see [Figure 33 on page 452](#)). The surface line is returned as a list of surface points in Cartesian coordinates (datasets `x, y`). For holes, the surface points are also given in polar coordinates (datasets `Radius, Theta`), measured relative to the fitted hole axis at the respective height z.

In addition, the extractor returns the coordinates of an ellipse fitted to the hole cross-section (datasets `x_fit, y_fit, Radius_fit`). If `output_type=tdr`, then the surface points are written to a TDR file for plotting in Sentaurus Visual. If `output_type=csv`, then the datasets are written to a CSV file with the same naming convention as for TDR files, but with the suffix `_surface.csv`.

- Extracted data can be returned by the `extract` command as a Tcl list, which is formatted in the following way:

```
// DOE parameters (scalar quantities)
{
    { Depth value1 }
    { Tilt   value2 }
    ...
}
// Datasets (1D z-dependent quantities)
{
    { Z           { value1 value2 value3 ... } }
    { Radius_Avg { value1 value2 value3 ... } }
```

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```
{ Radius_SD { value1 value2 value3 ... } }
...
}
// Surface points at given xy planes
{
{ Z { value1 value2 value3 ... } }
{ X { value1 value2 value3 ... } }
{ Y { value1 value2 value3 ... } }
...
}
```

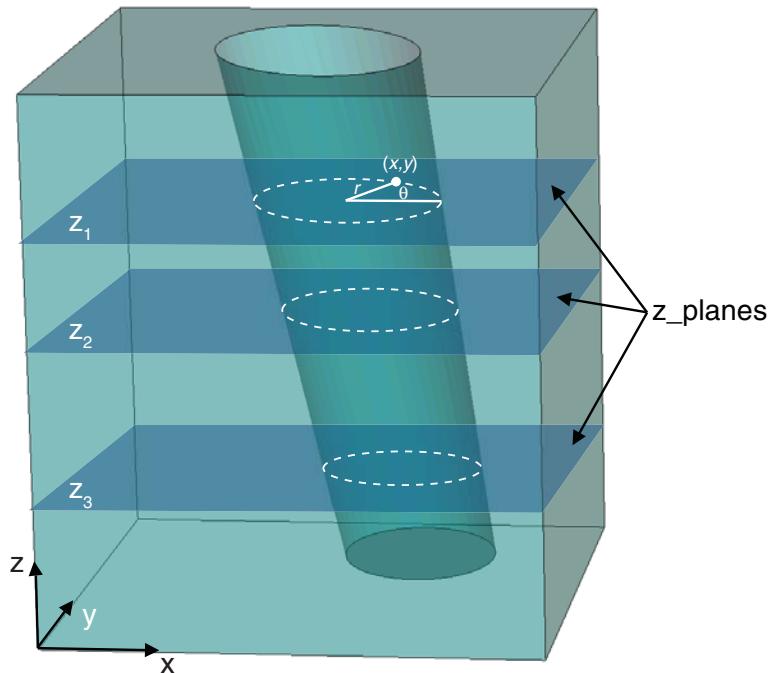
You can also write more than one output type simultaneously by setting `output_type` to a list of values. For example:

```
output_type={doe csv tdr}
```

If `output_type={}` is empty, no DOE or file output is generated; only the extracted data is returned as a Tcl list.

Depending on the size of the extraction window, more or fewer surface points of the structure are considered for the computation of the profile statistics. Therefore, by increasing the extraction window (for example, by increasing the distance between `point1` and `point2` for trenches in [Figure 32 on page 450](#)), statistical noise can be reduced, since more surface points are considered for the statistics.

Figure 33 Extracting surface points of a hole or trench in the xy plane at different heights z



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Depending on the morphology of the structure, it might also be useful to apply a smoothing on the profile data by setting the `smoothing_order` parameter.

Table 64 *DOE parameters for shape analysis*

DOE parameter	Description
Parameters common to both reference_shape=cylinder_hole and reference_shape=trench	
AxisCurvature_Avg	Average axis curvature along the z-axis
AxisCurvature_Max	Maximum axis curvature along the z-axis
AxisCurvature_Med	Median of the axis curvature along the z-axis
AxisCurvature_Min	Minimum axis curvature along the z-axis
AxisCurvature_SD	Standard deviation of the axis curvature along the z-axis
AxisOffset_Avg	Average axis offset along the z-axis
AxisOffset_Max	Maximum axis offset along the z-axis
AxisOffset_Med	Median of the axis offset along the z-axis
AxisOffset_Min	Minimum axis offset along the z-axis
AxisOffset_SD	Standard deviation of the axis offset along the z-axis
AxisTilt_Avg	Average axis tilt angle along the z-axis
AxisTilt_Max	Maximum axis tilt angle along the z-axis
AxisTilt_Med	Median of the axis tilt angle along the z-axis
AxisTilt_Min	Minimum axis tilt angle along the z-axis
AxisTilt_SD	Standard deviation of the axis tilt angle along the z-axis
Depth	Depth of the hole or trench
TiltTheta	Vertical slope of the fitted tilt axis (given by the angle between the tilt axis and the z-axis)
Z_AxisCurvature_Max	The z-coordinate of the maximum axis curvature
Z_AxisCurvature_Min	The z-coordinate of the minimum axis curvature

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Table 64 DOE parameters for shape analysis (Continued)

DOE parameter	Description
Z_AxisOffset_Max	The z-coordinate of the maximum axis offset along the z-axis
Z_AxisOffset_Min	The z-coordinate of the minimum axis offset along the z-axis
Z_AxisTilt_Max	The z-coordinate of the maximum tilt angle
Z_AxisTilt_Min	The z-coordinate of the minimum tilt angle
Z_Bottom	The z-coordinate at which the bottom of the hole or trench is measured. The measurement point can be shifted upwards by specifying <code>bottom_shift</code> in the <code>extract</code> command.
Z_Top	The z-coordinate at which the top of the hole or trench is measured. The measurement point can be shifted downwards by specifying <code>top_shift</code> in the <code>extract</code> command.
Parameters specific to reference_shape=cylinder_hole	
AxisOffsetPhi_Avg	Average direction of the axis offset along the z-axis (given by an angle ϕ relative to the x-axis)
AxisOffsetPhi_SD	Standard deviation of the axis offset direction along the z-axis
Eccentricity_Avg	Average eccentricity of the elliptic hole along the z-axis
Eccentricity_Max	Maximum eccentricity of the elliptic hole along the z-axis
Eccentricity_Med	Median of the eccentricity of the elliptic hole along the z-axis
Eccentricity_Min	Minimum eccentricity of the elliptic hole along the z-axis
Eccentricity_SD	Standard deviation of the eccentricity of the elliptic hole along the z-axis
EllipseRotation_Avg	Average angle between the major elliptic axis and the x-axis (the average is taken along the z-axis)
EllipseRotation_SD	Standard deviation of the angle between the major elliptic axis and the x-axis (measured along the z-axis)
FitRadius_Avg	Average fitted radius of the hole along the z-axis
FitRadius_Bottom	Average fitted radius at $z=Z_{\text{Bottom}}$

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Table 64 DOE parameters for shape analysis (Continued)

DOE parameter	Description
FitRadius_Max	Maximum fitted hole radius along the z-axis
FitRadius_Med	Median of the fitted hole radius along the z-axis
FitRadius_Min	Minimum fitted hole radius along the z-axis
FitRadius_SD	Standard deviation of the fitted hole radius along the z-axis
FitRadius_Top	Average fitted hole radius at $z=Z_{\text{Top}}$
MajorSemiaxis_Avg	Average major semi-axis of the elliptic hole along the z-axis
MajorSemiaxis_Max	Maximum major semi-axis of the elliptic hole along the z-axis
MajorSemiaxis_Med	Median of the major semi-axis of the elliptic hole along the z-axis
MajorSemiaxis_Min	Minimum major semi-axis of the elliptic hole along the z-axis
MajorSemiaxis_SD	Standard deviation of the major semi-axis of the elliptic hole along the z-axis
MinorSemiaxis_Avg	Average minor semi-axis of the elliptic hole along the z-axis
MinorSemiaxis_Max	Maximum minor semi-axis of the elliptic hole along the z-axis
MinorSemiaxis_Med	Median of the minor semi-axis of the elliptic hole along the z-axis
MinorSemiaxis_Min	Minimum minor semi-axis of the elliptic hole along the z-axis
MinorSemiaxis_SD	Standard deviation of the minor semi-axis of the elliptic hole along the z-axis
Phi_AxisOffset_Max	Direction of the maximum axis offset along the z-axis (given by an angle ϕ relative to the x-axis)
Phi_AxisOffset_Min	Direction of the minimum axis offset along the z-axis (given by an angle ϕ relative to the x-axis)
Radius_Avg	Average radius of the hole along the z-axis
Radius_Max	Maximum hole radius along the z-axis
Radius_Med	Median of the hole radius along the z-axis

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Table 64 DOE parameters for shape analysis (Continued)

DOE parameter	Description
Radius_Min	Minimum hole radius along the z-axis
Radius_SD	Standard deviation of the hole radius along the z-axis
TiltPhi	Orientation of the fitted tilt axis (given by an angle ϕ in the xy plane, measured relative to the x-axis)
Z_Eccentricity_Max	The z-coordinate of the maximum eccentricity of the elliptic hole
Z_Eccentricity_Min	The z-coordinate of the minimum eccentricity of the elliptic hole
Z_FitRadius_Max	The z-coordinate of the maximum fitted hole radius
Z_FitRadius_Min	The z-coordinate of the minimum fitted hole radius
Z_MajorSemiaxis_Max	The z-coordinate of the maximum major semi-axis of the elliptic hole
Z_MajorSemiaxis_Min	The z-coordinate of the minimum major semi-axis of the elliptic hole
Z_MinorSemiaxis_Max	The z-coordinate of the maximum minor semi-axis of the elliptic hole
Z_MinorSemiaxis_Min	The z-coordinate of the minimum minor semi-axis of the elliptic hole
Z_Radius_Max	The z-coordinate of the maximum hole radius
Z_Radius_Min	The z-coordinate of the minimum hole radius
Parameters specific to reference_shape=trench	
Halfwidth_Avg	Average distance between the user-defined trench center plane and the trench surface along the z-axis
Halfwidth_Max	Maximum distance between the user-defined trench center plane and the trench surface along the z-axis
Halfwidth_Med	Median distance between the user-defined trench center plane and the trench surface along the z-axis
Halfwidth_Min	Minimum distance between the user-defined trench center plane and the trench surface along the z-axis
Halfwidth_SD	Standard deviation of the distance between the user-defined trench center plane and the trench surface along the z-axis

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Table 64 DOE parameters for shape analysis (Continued)

DOE parameter	Description
LeftHalfwidth_Avg	Average distance between the user-defined trench center plane and the left trench surface along the z-axis
LeftHalfwidth_Max	Maximum distance between the user-defined trench center plane and the left trench surface along the z-axis
LeftHalfwidth_Med	Median distance between the user-defined trench center plane and the left trench surface along the z-axis
LeftHalfwidth_Min	Minimum distance between the user-defined trench center plane and the left trench surface along the z-axis
LeftHalfwidth_SD	Standard deviation of the distance between the user-defined trench center plane and the left trench surface along the z-axis
RightHalfwidth_Avg	Average distance between the user-defined trench center plane and the right trench surface along the z-axis
RightHalfwidth_Max	Maximum distance between the user-defined trench center plane and the right trench surface along the z-axis
RightHalfwidth_Med	Median distance between the user-defined trench center plane and the right trench surface along the z-axis
RightHalfwidth_Min	Minimum distance between the user-defined trench center plane and the right trench surface along the z-axis
RightHalfwidth_SD	Standard deviation of the distance between the user-defined trench center plane and the right trench surface along the z-axis
Width_Avg	Average width of the trench along the z-axis
Width_Bottom	Average width of the trench at $z=Z_{Bottom}$
Width_Max	Maximum width of the trench along the z-axis
Width_Med	Median width of the trench along the z-axis
Width_Min	Minimum width of the trench along the z-axis
Width_SD	Standard deviation of the width of the trench along the z-axis
Width_Top	Average width of the trench at $z=Z_{Top}$
Z_Halfwidth_Max	The z-coordinate of the maximum trench half-width

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Table 64 DOE parameters for shape analysis (Continued)

DOE parameter	Description
Z_Halfwidth_Min	The z-coordinate of the minimum trench half-width
Z_LeftHalfwidth_Max	The z-coordinate of the maximum left trench half-width
Z_LeftHalfwidth_Min	The z-coordinate of the minimum left trench half-width
Z_RightHalfwidth_Max	The z-coordinate of the maximum right trench half-width
Z_RightHalfwidth_Min	The z-coordinate of the minimum right trench half-width
Z_Width_Max	The z-coordinate of the maximum trench width
Z_Width_Min	The z-coordinate of the minimum trench width

Table 65 One-dimensional datasets for shape analysis

Parameter	Description
Parameters common to both reference_shape=cylinder_hole and reference_shape=trench	
AxisCurvature	Local curvature of the fitted center line
AxisTilt	Local slope angle of the fitted center line
SurfaceCoverage_<Material>_Avg	Surface coverage of material <Material> (averaged along the surface line at fixed height z). Note: This parameter can only be specified for PMC structures.
Thickness_<Material>_Avg	Thickness of the layer between the gas interface and the bulk interface of material <Material> (averaged along the surface line at fixed height z). Note: This parameter yields reasonable results only for closed material layers, such as thin deposited polymer layers covering the cylindrical hole surface. This parameter can only be specified for PMC structures.
Z	The z-coordinate

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Table 65 One-dimensional datasets for shape analysis (Continued)

Parameter	Description
Parameters specific to reference_shape=cylinder_hole	
AxisOffsetPhi	Direction of the shift of the fitted hole center from the cylinder axis as a function of z
AxisOffsetR	Distance between the fitted hole center and the cylinder axis as a function of z
AxisOffsetX	The x-shift of the fitted hole center from the cylinder axis as a function of z
AxisOffsetY	The y-shift of the fitted hole center from the cylinder axis as a function of z
Eccentricity	Eccentricity of the ellipse (fitted from the surface line at each height z). The eccentricity is defined by: $\text{Eccentricity} = \frac{\text{MajorSemiaxis} - \text{MinorSemiaxis}}{\text{MajorSemiaxis} + \text{MinorSemiaxis}}$
EllipseRotation	Angle between the major semi-axis of the fitted ellipse and the x-axis (fitted from the surface line at each height z)
FitRadius_Avg	Average distance between the fitted hole center and the hole surface (averaged along the surface line at fixed height z)
FitRadius_Max	Maximum distance between the fitted hole center and the hole surface (measured along the surface line at fixed height z)
FitRadius_Min	Minimum distance between the fitted hole center and the hole surface (measured along the surface line at fixed height z)
FitRadius_SD	Standard deviation of the distance between the fitted hole center and the hole surface (taken along the surface line at fixed height z)
MajorSemiaxis	Major semi-axis of the ellipse (fitted from the surface line at each height z)
MinorSemiaxis	Minor semi-axis of the ellipse (fitted from the surface line at each height z)

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Table 65 One-dimensional datasets for shape analysis (Continued)

Parameter	Description
Radius_Avg	Average distance between the cylinder axis and the hole surface (averaged along the surface line at fixed height z)
Radius_Max	Maximum distance between the cylinder axis and the hole surface (measured along the surface line at fixed height z)
Radius_Min	Minimum distance between the cylinder axis and the hole surface (measured along the surface line at fixed height z)
Radius_SD	Standard deviation of the distance between the cylinder axis and the hole surface (taken along the surface line at fixed height z)
z	The z-coordinate
Parameters specific to reference_shape=trench	
AxisOffset	Distance between the fitted trench center and the user-defined trench axis as function of z
Halfwidth_Avg	Average half-width of the trench (averaged along the surface points at fixed height z)
Halfwidth_Max	Maximum half-width of the trench (averaged along the surface points at fixed height z)
Halfwidth_Min	Minimum half-width of the trench (averaged along the surface points at fixed height z)
Halfwidth_SD	Standard deviation of the half-width of the trench (averaged along the surface points at fixed height z)
LeftHalfwidth_Avg	Average left half-width of the trench (averaged along the surface points at fixed height z)
LeftHalfwidth_Max	Maximum left half-width of the trench (averaged along the surface points at fixed height z)
LeftHalfwidth_Min	Minimum left half-width of the trench (averaged along the surface points at fixed height z)
LeftHalfwidth_SD	Standard deviation of the left half-width of the trench (averaged along the surface points at fixed height z)

Table 65 One-dimensional datasets for shape analysis (Continued)

Parameter	Description
RightHalfwidth_Avg	Average right half-width of the trench (averaged along the surface points at fixed height z)
RightHalfwidth_Max	Maximum right half-width of the trench (averaged along the surface points at fixed height z)
RightHalfwidth_Min	Minimum right half-width of the trench (averaged along the surface points at fixed height z)
RightHalfwidth_SD	Standard deviation of the right half-width of the trench (averaged along the surface points at fixed height z)
Width_Avg	Average width of the trench (averaged along the surface points at fixed height z)
Width_Max	Maximum width of the trench (averaged along the surface points at fixed height z)
Width_Min	Minimum width of the trench (averaged along the surface points at fixed height z)
Width_SD	Standard deviation of the width of the trench (averaged along the surface points at fixed height z)

Cylindrical Hole Profile

```
extract type=cylinder_hole_profile center=<v> point_max=<v> \
point_min=<v> \
[file=<c>] [structure=<c>]
```

When specifying `type=cylinder_hole_profile`, the vertical profile of a cylindrical hole is extracted from a PMC structure. The `structure` parameter must denote a PMC structure. The values specified with the parameters `point_max` and `point_min` define a cuboid within which, for each vertical coordinate, the average, the maximum, and the minimum radius and the standard deviation of the radius are extracted.

The extracted values are written to a file in comma-separated value (CSV) format. By default, the file name is the base name of the command file and it uses the suffix `_cyl.csv`. Alternatively, a file name can be specified with the parameter `file`. The resulting file can be visualized in Sentaurus Visual or other visualization tools.

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Bounding Box of Materials and Regions

To extract the bounding box of regions having any of the specified materials, use the command:

```
extract type=bounding_box \
[materials=<l>] [name=<c>] [silent=<b>] [structure=<c>]
```

This command returns the bounding box of regions of the given structure that have any of the specified materials. If no materials are specified, the bounding box of the entire structure is returned. If the list of materials is not empty but contains only materials that are not present in the specified structure, an error is issued.

To extract the bounding box of regions having any of the specified names, use the command:

```
extract type=bounding_box \
[name=<c>] [regions=<l>] [silent=<b>] [structure=<c>]
```

This command returns the bounding box of regions of the given structure that have any of the specified region names. If no regions are specified, the bounding box of the entire structure is returned. If the list of regions is not empty but contains only regions that are not present in the specified structure, an error is issued.

Note:

When the structure specified with the `structure` parameter is a PMC structure, the list of region names must be empty.

Vertical Coordinates of the Top and Bottom of the Bounding Box of Materials and Regions

To extract the bottom coordinate of the bounding box of the regions of a structure having any of the specified materials, use the command:

```
extract type=bounding_box_bottom \
[materials=<l>] [name=<c>] [silent=<b>] [structure=<c>]
```

This command returns the vertical coordinate of the bottom of the bounding box of regions of the given structure that have any of the specified materials. If no materials are specified, the vertical coordinate of the bottom of the bounding box of the entire structure is returned. If the list of materials is not empty but contains only materials that are not present in the specified structure, an error is issued.

Note:

When the structure specified with the `structure` parameter is a PMC structure, the list of materials must be empty.

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To extract the top coordinate of the bounding box of the regions of a structure having any of the specified materials, use the command:

```
extract type=bounding_box_top \
[materials=<l>] [name=<c>] [silent=<b>] [structure=<c>]
```

This command returns the vertical coordinate of the top of the bounding box of regions of the given structure that have any of the specified materials. If no materials are specified, the vertical coordinate of the top of the bounding box of the entire structure is returned.

If the list of materials is not empty but contains only materials that are not present in the specified structure, an error is issued.

Note:

When the structure specified with the `structure` parameter is a PMC structure, the list of materials must be empty.

To extract the bottom coordinate of the bounding box of the regions of a boundary structure having any of the specified names, use the command:

```
extract type=bounding_box_bottom \
[name=<c>] [regions=<l>] [silent=<b>] [structure=<c>]
```

This command returns the vertical coordinate of the bottom of the bounding box of regions of the given structure that have any of the specified region names. The structure specified by the parameter `structure` must be a boundary structure. If no region names are specified, the vertical coordinate of the bottom of the bounding box of the entire structure is returned. If the list of region names is not empty but contains only regions that are not present in the specified structure, an error is issued.

To extract the top coordinate of the bounding box of the regions of a boundary structure having any of the specified names, use the command:

```
extract type=bounding_box_top \
[name=<c>] [regions=<l>] [silent=<b>] [structure=<c>]
```

This command returns the vertical coordinate of the top of the bounding box of regions of the given structure that have any of the specified region names. The structure specified by the parameter `structure` must be a boundary structure. If no region names are specified, the vertical coordinate of the top of the bounding box of the entire structure is returned. If the list of region names is not empty but contains only regions that are not present in the specified structure, an error is issued.

Dimension of Structure

To extract of the dimension of a structure, use the command:

```
extract type=dimension [name=<c>] [silent=<b>] [structure=<c>]
```

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Note:

This extraction type supports both boundary structures and PMC structures.

Example: dimension

```
extract type=dimension
```

This command extracts and outputs the dimension of the processed structure.

Damage Integral

```
extract type=damage_integral [name=<c>] [point_max=<v>] \
[point_min=<v>] [structure=<c>]
```

Damage is integrated over the entire structure or, if specified, a box defined by `point_min` and `point_max`. The damage value is multiplied by the cell volume for each cell, where the volume is in cm³.

Surface Coverage

```
extract type=surface_coverage [point_max=<v>] [point_min=<v>] \
[silent=<b>] [species=<l>] [structure=<c>]
```

For PMC structures, the command extracts the surface coverage fraction from a list of species bounded by `point_min` and `point_max`, if given. If you do not specify a species list, then the command returns the surface coverage of all species. Similarly, if you do not specify `point_min` and `point_max`, then the command returns the surface coverage of the entire structure. The command returns a Tcl list of {<species> <fraction>} lists, where <fraction> is a number between 0 and 1. For example:

```
set coverages [extract type=surface_coverage species={Si Ge}]

foreach spec_val $coverages {
    puts "species: [lindex $spec_val 0], value: [lindex $spec_val 1]"
}
```

Note:

When you start Sentaurus Topography 3D with the `--processes` command-line option with a value greater than 1 (see [Table 1 on page 18](#)), the parameter `structure` must not denote a structure obtained from the `etch` command using `method=pmc averaging_runs=1`.

Structure Spacing

To extract the spacing of a PMC or GC structure, use the command:

```
extract type=spacing [structure=<c>]
```

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Note:

This extraction type supports only PMC and GC structures.

Structure Type

To extract the type of a structure, use the command:

```
extract type=structure_type [structure=<c>]
```

This command returns the type of the given structure. Possible outputs are:

- brep (for boundary structures)
- gc (for GC structures)
- pmc (for PMC structures)

Table 66 Parameters of extract command

Parameter	Description
axis	Sets the direction of one of the coordinate axes. Options are: <ul style="list-style-type: none">• x• y• z Type: Character Default: none
bottom_shift	Sets the distance above the structure bottom, along the vertical z-axis, where the bottom width or radius is measured. Note: You can specify this parameter only if type=shape_analysis. Type: Number Default: 0 Range: [0 , ∞[Unit: μm
center	Sets the 2D position of the vertical extraction axis. Type: Vector Default: none Unit: μm

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Table 66 Parameters of extract command (Continued)

Parameter	Description
csv_file	<p>Sets the name of a CSV file.</p> <p>Note: You can only specify this parameter if <code>output_type=csv</code>.</p> <p>Type: Character Default: <code><basename>_extract.csv</code></p>
direction	<p>Sets the direction of the cutting line.</p> <p>Type: Vector Default: none</p>
doe_parameters	<p>Sets a list of DOE parameter names to be shown as output in Sentaurus Workbench.</p> <p>Note: You can specify this parameter only if <code>output_type=doe</code> and <code>type=shape_analysis</code>.</p> <p>Type: List Default: By default, all DOE parameters are shown; Table 64 lists possible DOE parameter names</p>
exposed_only	<p>Specifies whether only the exposed materials, regions, or region parts must be extracted.</p> <p>Type: Boolean Default: false</p>
extract_surface	<p>Specifies whether to extract the surface line around the hole axis at given xy planes. The z-positions of the xy planes can be specified by the parameter <code>z_planes</code>.</p> <p>Note: You can specify this parameter only if <code>type=shape_analysis</code>.</p> <p>Type: Boolean Default: false</p>
file	<p>Sets the name of the file in which the extracted information is saved.</p> <p>Type: Character Default: <code><basename>_extract.tdr</code></p>

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Table 66 Parameters of extract command (Continued)

Parameter	Description
interface	<p>Sets a pair of species names that specify the material interface at which the DOE parameters must be measured.</p> <p>Note:</p> <p>For this parameter:</p> <ul style="list-style-type: none">Only layers containing the specified material interface are extracted. This might produce meaningless results for some DOE parameters such as <code>Depth</code>, <code>Z_Bottom</code>, and <code>Z_Top</code>.You can specify this parameter only for PMC structures and if <code>type=shape_analysis</code>. <p>Type: List</p> <p>Default: none</p>
material1	<p>Sets the name of a material.</p> <p>Type: Character</p> <p>Default: none</p>
material2	<p>Sets the name of a material.</p> <p>Type: Character</p> <p>Default: none</p>
materials	<p>Sets the list of materials to consider for the extraction when any of the following are specified:</p> <ul style="list-style-type: none"><code>type=bounding_box</code><code>type=bounding_box_bottom</code><code>type=bounding_box_top</code><code>type=probe</code> <p>When using <code>type=probe</code>, any edge found along the specified line that lies in a region having a material not included in the list will be ignored and will not be included in the result. If <code>materials</code> is omitted, any material will be included in the output.</p> <p>Note:</p> <p>When <code>type=probe</code>, you can specify <code>materials</code> only if <code>property=length</code>.</p> <p>Type: List</p> <p>Default: none</p>

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Table 66 Parameters of extract command (Continued)

Parameter	Description
max_depth	<p>Sets the maximum depth of the cuboid bounding box used for extraction (see Figure 32 on page 450).</p> <p>Note: You can specify this parameter only if <code>type=shape_analysis</code> and <code>reference_shape=trench</code>.</p> <p>Type: Number Default: none Range:]0, ∞[Unit: µm</p>
max_radius	<p>Sets the radius of the cylindrical bounding box used for extraction (see Figure 32).</p> <p>Note: You can specify this parameter only if <code>type=shape_analysis</code> and <code>reference_shape=cylinder_hole</code>.</p> <p>Type: Number Default: none Range:]0, ∞[Unit: µm</p>
max_width	<p>Sets the maximum width of the cuboid bounding box used for extraction (see Figure 32 on page 450).</p> <p>Note: You can specify this parameter only if <code>type=shape_analysis</code> and <code>reference_shape=trench</code>.</p> <p>Type: Number Default: none Range:]0, ∞[Unit: µm</p>

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Table 66 Parameters of extract command (Continued)

Parameter	Description
name	<p>Sets the name of the extraction.</p> <p>Note: If <code>type=shape_analysis</code>, the name is prepended to the DOE parameter name to uniquely identify the extraction.</p> <p>Type: Character Default: Hole<counter> (if <code>reference_shape= cylinder_hole</code>) <code>Trench<counter></code> (if <code>reference_shape= trench</code>) <counter> is an integer that uniquely identifies the extraction. If <code>counter=0</code>, the DOE prefix is omitted.</p>
normal	<p>Sets the normal of the specified plane.</p> <p>Type: Vector Default: none</p>
output	<p>Sets a filtering option. Options are:</p> <ul style="list-style-type: none"> • all • first • inside • last • outside <p>The values <code>inside</code> and <code>outside</code> only apply if a cutting line is specified with the <code>point1</code> and <code>point2</code> parameters.</p> <p>Type: Character Default: all</p>
output_type	<p>Sets the output of extracted data. Options are:</p> <ul style="list-style-type: none"> • <empty>: If you specify <code>output_type={}</code>, no DOE or file output is generated; the extracted data is returned as a Tcl list. • csv: Writes datasets in a tabular format to a CSV file specified by the <code>csv_file</code> parameter. • doe: Returns scalar quantities to Sentaurus Workbench as DOE parameters. • tdr: Writes datasets to a TDR file specified by the <code>tdr_file</code> parameter. <p>Note: You can specify the parameter <code>output_type</code> only if <code>type=shape_analysis</code>.</p> <p>Type: Character Default: doe</p>

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Table 66 Parameters of extract command (Continued)

Parameter	Description
point	<p>Sets a point on the cutting line or the cutting plane.</p> <p>Note: The dimension of this point must match the dimension of the structure for which it is used.</p> <p>Type: Vector Default: none Unit: μm</p>
point_max	<p>Sets the maximum corner point of the cuboid.</p> <p>Type: Vector Default: none Unit: μm</p>
point_min	<p>Sets the minimum corner point of the cuboid.</p> <p>Type: Vector Default: none Unit: μm</p>
point1	<p>If defining an extraction line, sets the first point on the cutting line or the cutting plane.</p> <p>Note: The dimension of this point must match the dimension of the structure for which it is used.</p> <p>When used for shape analysis (<code>type=shape_analysis</code>):</p> <ul style="list-style-type: none"> • If <code>reference_shape=cylinder_hole</code>, <code>point1</code> specifies the first vertex of the axis of the cylindrical bounding box for extraction (see Figure 32 on page 450 (left)). • If <code>reference_shape=trench</code>, <code>point1</code> is the first vertex of the trench orientation vector, defined at the top of the cuboid bounding box for extraction (see Figure 32 (right)). <p>Type: Vector Default: none Unit: μm</p>

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Table 66 Parameters of extract command (Continued)

Parameter	Description
point2	<p>If defining an extraction line, sets the second point on the cutting line or the cutting plane.</p> <p>Note: The dimension of this point must match the dimension of the structure for which it is used.</p> <p>When used for shape analysis (<code>type=shape_analysis</code>):</p> <ul style="list-style-type: none"> • If <code>reference_shape=cylinder_hole</code>, <code>point2</code> specifies the second vertex of the axis of the cylindrical bounding box for extraction (see Figure 32 on page 450 (left)). • If <code>reference_shape=trench</code>, <code>point2</code> is the second vertex of the trench orientation vector, defined at the top of the cuboid bounding box for extraction (see Figure 32 (right)). <p>Type: Vector Default: none Unit: µm</p>
point3	<p>Sets a third point on the cutting plane.</p> <p>Type: Vector Default: none Unit: µm</p>
position	<p>Sets the cutting plane distance from the origin measured in the direction defined by <code>axis</code>.</p> <p>Type: Number Default: none Unit: µm</p>
probe_empty_space	<p>Specifies whether to probe empty space.</p> <p>Note: You can specify this parameter only if <code>property=length</code>.</p> <p>Type: Boolean Default: false</p>

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Table 66 Parameters of extract command (Continued)

Parameter	Description
property	Sets the property to be associated with segments returned by type=probe. Options are: <ul style="list-style-type: none"> • length • material • region • region_part Type: Character Default: material
reference_shape	Sets the reference shape to be used for shape analysis. Options are: <ul style="list-style-type: none"> • cylinder_hole • trench Note: You can specify this parameter only if type=shape_analysis. Type: Character Default: none
region	Sets the name of the region for which properties are extracted. Type: Character Default: none
region_1	Sets the name of the region on the first side of the interface for which the area is extracted. Type: Character Default: none
region_2	Sets the name of the region on the second side of the interface for which the area is extracted. Type: Character Default: none
region_part1	Sets the name of a region and the name of a part of that region, given in the format: {region_name part_name} Type: List Default: none
region_part2	Sets the name of a region and the name of a part of that region, given in the format: {region_name part_name} Type: List Default: none

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Table 66 Parameters of extract command (Continued)

Parameter	Description
region1	Sets the name of a region. Type: Character Default: none
region2	Sets the name of a region. Type: Character Default: none
regions	Sets the list of regions to consider when any of the following are specified: <ul style="list-style-type: none"> • type=bounding_box • type=bounding_box_bottom • type=bounding_box_top Type: List Default: none
silent	This parameter can be used with all extraction types to control whether or not the extracted values are written to the log file. When <code>silent=true</code> , the extracted values are not written to the log file, but they can be assigned to a Tcl variable. Type: Boolean Default: false
smoothing_order	Sets the order of the smoothing filter (Savitzky–Golay filter). If <code>smoothing_order=0</code> , smoothing is switched off. Note: You can specify this parameter only if <code>type=shape_analysis</code> . Type: Number Default: 0 Range: [0, 5, 7, 9, 11, 13, 15, 17, 19, 21, 23, 25]
species	Specifies a list of species for which the surface coverage is extracted. Type: List Default: none
structure	Sets the name of the structure whose properties must be extracted. Type: Character Default: default_structure

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Table 66 Parameters of extract command (Continued)

Parameter	Description
tdr_file	<p>Sets the name of a TDR file.</p> <p>Note: You can specify this parameter only if <code>output_type=tdr</code> and <code>type=shape_analysis</code>.</p> <p>Type: Character Default: <basename>.extract.tdr</p>
top_shift	<p>Sets the distance below the structure top, along the vertical z-axis, where the top width or radius is measured.</p> <p>Note: You can specify this parameter only if <code>type=shape_analysis</code>.</p> <p>Type: Number Default: 0 Range:]0, ∞[Unit: μm</p>
type	<p>Sets the extraction type. Table 67 lists the extraction types and summarizes which structure types are supported for the different extraction types.</p> <p>Note: You can use <code>type=cylinder_hole_profile</code> only for structures resulting from simulations that used the PMC method.</p> <p>Type: Character Default: none</p>
vertical_spacing	<p>Sets the vertical spacing to use when scanning the structure in the vertical direction during shape analysis.</p> <p>This parameter can only be specified for brep structures, and it is mandatory only if there is no preceding level-set etching or deposition step.</p> <p>Type: Number Default: Vertical spacing of the last preceding etching or deposition step Range:]0, ∞[Unit: μm</p>

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Table 66 Parameters of extract command (Continued)

Parameter	Description
z_planes	<p>Sets the z-values of the xy planes, on which the surface line of the hole should be extracted.</p> <p>Note: You can specify this parameter only if <code>extract_surface=true</code>.</p> <p>Type: List Default: none Range: $]-\infty, \infty[$ Unit: μm</p>

Table 67 Supported structure types for different extraction types

Extraction type	Boundary structure	PMC structure
1d_cut	Supported	Supported
2d_cut	Supported	Not supported
area	Supported	Not supported
bottom_exposed	Supported	Supported
bounding_box	Supported	Supported when parameters <code>materials</code> and <code>regions</code> are empty
bounding_box_bottom	Supported	Supported when parameters <code>materials</code> and <code>regions</code> are empty
bounding_box_exposed	Supported	Supported when parameters <code>materials</code> and <code>regions</code> are empty
bounding_box_top	Supported	Not supported
cylinder_hole_profile	Not supported	Supported
damage_integral	Not supported	Supported
dimension	Supported	Supported
interface	Supported	Supported only when using parameters <code>material1</code> and <code>material2</code>

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Table 67 *Supported structure types for different extraction types (Continued)*

Extraction type	Boundary structure	PMC structure
interface_area	Supported	Not supported
material_name	Supported	Not supported
material_names	Supported	Supported only when exposed_only=false
part_area	Supported	Not supported
part_volume	Supported	Not supported
probe	Supported	Supported only when property=length or property=material
region_names	Supported	Not supported
region_parts	Supported	Not supported
shape_analysis	Supported	Supported
shortest_distance	Supported	Not supported
slice	Supported	Supported
spacing	Not supported	Supported
structure_type	Supported	Supported
surface_coverage	Not supported	Supported
top_exposed	Supported	Supported
volume	Supported	Not supported

fill

This command performs one fill operation or multiple fill operations sequentially. A fill operation can be performed in either the vertical upward direction or the vertical downward direction.

A fill operation in the vertical upward direction consists of filling a structure with a material up to a certain height, measured from the top of the structure. A fill operation in the vertical upward direction is similar to a deposition followed by a planarization step.

A fill operation in the vertical downward direction consists of adding, under the structure, a layer with the same cross section as the structure and of a certain height, measured from the bottom of the structure. The bottom of the added layer is flat and parallel to the bottom of the structure.

Note:

When you start Sentaurus Topography 3D with the `--processes` command-line option with a value greater than 1 (see [Table 1 on page 18](#)), the parameter `structure` must not denote a structure obtained from the `etch` command using `method=pmc averaging_runs=1`.

Syntax

Fill a boundary structure:

```
fill material=<l> thickness=<v> \
[accuracy=<n>] [comment=<c>] [decimate=<b>] [direction=<c>] \
[merge=<b>] [min_angle=<n>] [min_dihedral_angle=<n>] \
[region=<c>] [ridge_angle=<n>] [shortest_edge=<n>] \
[structure=<c>] [times=<n>]
```

Fill a PMC structure:

```
fill material=<l> thickness=<v> \
[comment=<c>] [direction=<c>] [structure=<c>] [times=<n>]
```

Chapter 6: Input Commands

fill

Table 68 Parameters of *fill* command

Parameter	Description
accuracy	<p>Sets the maximum deviation between the decimated surface of the boundary structure produced by Boolean operations and its original surface.</p> <p>When set to -1, the used value is half of the structure-dependent spacing epsilon¹.</p> <p>It can be specified only if both of the following conditions are met:</p> <ul style="list-style-type: none">• <code>structure</code> denotes a boundary structure.• <code>decimate=true</code>, or you do not specify the <code>decimate</code> parameter and specify <code>let decimate=true</code>. <p>Type: Number Default: Value set by <code>let decimate_accuracy=<n></code> Range: $\{-1\} \cup [0, \infty[$ Unit: μm</p>
comment	<p>Sets a comment for this process step that will be displayed or written to the log file.</p> <p>Type: Character Default: empty string</p>
decimate	<p>Specifies whether to decimate the boundary structure produced by Boolean operations.</p> <p>It can be specified only if <code>structure</code> denotes a boundary structure.</p> <p>Type: Boolean Default: Value set by <code>let decimate=</code></p>
direction	<p>The direction in which to deposit the specified materials. Options are:</p> <ul style="list-style-type: none">• up• down <p>Type: Character Default: up</p>

Chapter 6: Input Commands

fill

Table 68 Parameters of fill command (Continued)

Parameter	Description
material	<p>When <code>direction=up</code>, this parameter sets the materials with which to fill the structure. The structure is filled with the i-th material of parameter <code>material</code> up to the height specified by the i-th element of parameter <code>thickness</code>. If more than one material is specified, then none of them can be gas.</p> <p>When <code>direction=down</code>, this parameter sets the materials of the layers to add under the structure. Each added layer will have the same cross section as the structure to which it is added. The i-th element of parameter <code>material</code> specifies the material of the i-th added layer. The i-th element of parameter <code>thickness</code> specifies the thickness of the i-th added layer. The added layers are numbered in a downward direction: The first element of parameter <code>material</code> refers to the topmost layer and its last element refers to the bottommost layer. No specified material can be gas.</p> <p>Note: The number of elements of parameter <code>material</code> must equal those of parameter <code>thickness</code>.</p> <p>Type: List Default: none</p>
merge	<p>If set to <code>true</code>, the deposited region merges with the already existing regions of the same material in the structure.</p> <p>It can be specified only if <code>structure</code> denotes a boundary structure.</p> <p>Type: Boolean Default: false</p>
min_angle	<p>Sets the smallest angle in the elements of the decimated surface of the boundary structure produced by Boolean operations.</p> <p>It can be specified only if both of the following conditions are met:</p> <ul style="list-style-type: none"> • <code>structure</code> denotes a boundary structure. • <code>decimate=true</code>, or you do not specify the <code>decimate</code> parameter and specify <code>let decimate=true</code>. <p>Type: Number Default: Value set by <code>let decimate_min_angle=<n></code> Range: [0, 180] Unit: degree</p>

Chapter 6: Input Commands

fill

Table 68 Parameters of fill command (Continued)

Parameter	Description
min_dihedral_angle	<p>Sets the smallest dihedral angle between two elements of the decimated surface of the boundary structure produced by Boolean operations that share an edge.</p> <p>It can be specified only if both of the following conditions are met:</p> <ul style="list-style-type: none"> • <code>structure</code> denotes a boundary structure. • <code>decimate=true</code>, or you do not specify the <code>decimate</code> parameter and specify <code>let decimate=true</code>. <p>Type: Number Default: Value set by <code>let decimate_min_dihedral_angle=<n></code> Range: [0, 180] Unit: degree</p>
region	<p>Sets the name of the first region that is deposited.</p> <p>It can be specified only if <code>structure</code> denotes a boundary structure.</p> <p>Type: Character Default: none</p>
ridge_angle	<p>Sets the angle used by the decimation algorithm to determine geometric features of the boundary structure produced by Boolean operations.</p> <p>It can be specified only if both of the following conditions are met:</p> <ul style="list-style-type: none"> • <code>structure</code> denotes a boundary structure. • <code>decimate=true</code>, or you do not specify the <code>decimate</code> parameter and specify <code>let decimate=true</code>. <p>Type: Number Default: Value set by <code>let decimate_ridge_angle=<n></code> Range: [0, 180] Unit: degree</p>
shortest_edge	<p>Sets the shortest edge of the decimated surface of the boundary structure produced by Boolean operations.</p> <p>When set to -1, the used value is half of the structure-dependent spacing <code>epsilon</code>¹.</p> <p>It can be specified only if both of the following conditions are met:</p> <ul style="list-style-type: none"> • <code>structure</code> denotes a boundary structure. • <code>decimate=true</code>, or you do not specify the <code>decimate</code> parameter and specify <code>let decimate=true</code>. <p>Type: Number Default: Value set by <code>let decimate_shortest_edge=<n></code> Range: {-1} \cup [0, ∞[Unit: μm</p>

Chapter 6: Input Commands

fill

Table 68 Parameters of fill command (Continued)

Parameter	Description
structure	<p>Sets the name of the structure that must be filled.</p> <p>Note: This parameter cannot specify a PMC structure. To process such a structure, an explicit conversion of the structure is needed before calling the <code>fill</code> command (see Integration With Other Sentaurus Topography 3D Functionality on page 580).</p> <p>Type: Character Default: <code>default_structure</code></p>
thickness	<p>When <code>direction=up</code>, this parameter sets the thicknesses of the materials with which the structure is filled. The structure is filled with the i-th material of parameter <code>material</code> up to the height specified by the i-th element of parameter <code>thickness</code>.</p> <p>When <code>direction=down</code>, this parameter sets the thicknesses of the layers to add under the structure. Each added layer will have the same cross section as the structure to which it is added. The i-th element of parameter <code>thickness</code> specifies the thickness of the i-th added layer. The i-th element of parameter <code>material</code> specifies the material of the i-th added layer. The added layers are numbered in a downward direction: The first element of parameter <code>thickness</code> refers to the topmost layer and its last element refers to the bottommost layer.</p> <p>Note: The number of elements of parameter <code>thickness</code> must equal those of parameter <code>material</code>.</p> <p>Type: Vector Default: none Range: Each element of the vector must be in the range $[0, \infty[$ Unit: μm</p>
times	<p>Sets how many times the structure must be filled with the specified materials.</p> <p>Type: Number Default: 1 Range: $[1, 2147483647]$</p>

1. The structure-dependent spacing `epsilon` is logged out when defining a structure using the `define_structure` command.

Chapter 6: Input Commands

fill

Examples

```
fill material=Oxide thickness=0.5 comment="oxide fill" \
      region="filled_oxide"
```

This command deposits a region consisting of material Oxide, with a thickness of 0.5 μm . The thickness is measured from the top of the existing structure. The comment for this process step is displayed in the log file, and the region name is set to filled_oxide.

```
define_structure material=Silicon point_min={0 0 0} \
                  point_max={1 1 1}
fill material={Oxide Nitride} thickness={0.1 0.2} times=100
```

This command deposits a stack of 200 layers on a silicon substrate. The materials of the layers are Oxide and Nitride, alternating. The thickness of all Oxide layers is 0.1 μm ; the thickness of all Nitride layers is 0.2 μm .

```
fill material=Silicon thickness=1 direction=down
```

This command deposits a 1 μm -thick silicon layer under the structure to which it is applied.

Chapter 6: Input Commands

filter_structure

filter_structure

This command performs different operations.

Syntax

Execute Boolean operations:

```
filter_structure type=boolean \
[body=<c>] [boolean_accuracy=<n>] [decimate=<b>] \
[deposit_material=<c>] [min_angle=<n>] \
[min_dihedral_angle=<n>] [name=<c>] \
[ridge_angle=<n>] \
[shortest_edge=<n>] [structure=<c>] [surface_accuracy=<n>] \
[surface_decimate=<c>] [surface_min_angle=<n>] \
[surface_min_dihedral_angle=<n>] [surface_ridge_angle=<n>] \
[surface_shortest_edge=<n>]
```

Convert a boundary structure to a PMC structure. If you specify `split_replacements`, then split the specified compound materials into constituent species according to the material replacement map or maps specified in `split_replacements` and defined in the `define_material_replacement` command:

```
filter_structure type=convert_to_pmc spacing=<n> \
[name=<c>] [split_replacements=<l>] [structure=<c>] \
[top_gas_thickness=<n>]
```

Note:

This conversion is not available for 2D structures.

Create a copy of an existing structure:

```
filter_structure type=copy [name=<c>] [structure=<c>]
```

Convert a PMC structure to a boundary structure by using the dual-contouring method:

```
filter_structure type=dc \
[dc_min_angle=<n>] [dc_min_dihedral_angle=<n>] \
[dc_reference_volume_scaling=<n>] [dc_snap_to_box=<b>] \
[dc_version=<n>] [include_grain_index=<b>] \
[keep_top_gas=<b>] [mean_spacing=<n>]
```

Decimate the number of surface elements of a boundary structure:

```
filter_structure type=decimate tolerance=<n> \
[mean_spacing=<n>] [min_angle=<n>] [min_dihedral_angle=<n>] \
[name=<c>] [ridge_angle=<n>] \
[shortest_edge=<n>] [structure=<c>]
```

Chapter 6: Input Commands

filter_structure

Merge several regions of a boundary structure that have the same material into one region:

```
filter_structure type=merge_regions new_region_name=<c> \
merged_regions=<l> \
[name=<c>] [structure=<c>]
```

Create a boundary structure with a different surface discretization (not available for 2D structures):

```
filter_structure type=rediscretize_boundary \
[dc_min_angle=<n>] [dc_min_dihedral_angle=<n>] \
[decimate=<b>] [accuracy=<n>] [method=<c>] [min_angle=<n>] \
[min_dihedral_angle=<n>] [ridge_angle=<n>] [shortest_edge=<n>]] \
[material_priority=<l>] [material_selection=<c>] \
[mean_spacing=<n>] [structure=<c>]
```

Remove accumulated damage from a PMC structure:

```
filter_structure type=remove_damage [name=<c>] [structure=<c>]
```

Remove those parts from a boundary structure that are completely surrounded by gas and, therefore, are disconnected topologically from the bulk (see [Figure 34 on page 499](#)):

```
filter_structure type=remove_disconnected_top_parts \
[name=<c>] [structure=<c>]
```

Remove those parts from a boundary structure that fit the specified criteria of material, maximum area or maximum volume, materials in contact, and bounding box:

```
filter_structure type=remove_parts [exposed_only=<b>] \
[materials=<l>] [materials_in_contact=<l>] \
[maximum_area=<n>] [maximum_volume=<n>] \
[name=<c>] [point_max=<v>] [point_min=<v>] [silent=<b>] \
[structure=<c>]
```

Remove those parts from a PMC structure that fit the specified criterion of maximum volume:

```
filter_structure type=remove_parts maximum_volume=<n> \
[name=<c>] [silent=<b>] [structure=<c>]
```

Remove a region from a boundary structure:

```
filter_structure type=remove_region region=<c> \
[name=<c>] [structure=<c>]
```

Rename a region of a boundary structure:

```
filter_structure type=rename_region new_region_name=<c> \
region=<c> [name=<c>] [structure=<c>]
```

Chapter 6: Input Commands

filter_structure

Replace the material of a region in a boundary structure:

```
filter_structure type=replace_material region=<c> \
    new_material=<c> [name=<c>] [structure=<c>]
```

Replace a material in all matching regions of a boundary structure:

```
filter_structure type=replace_material \
    material=<c> new_material=<c> \
    [name=<c>] [structure=<c>]
```

Split specified compound materials in a PMC structure into constituent species according to a material replacement map or maps specified with `split_replacements` and defined in the `define_material_replacement` command:

```
filter_structure type=replace_material split_replacements=<l> \
    [name=<c>] [structure=<c>]
```

Convert materials in a PMC structure by mapping mixed PMC cells to compound materials (the map or maps specified in `merge_replacements` are created in the `define_material_replacement` command):

```
filter_structure type=replace_material merge_replacements=<l> \
    merge_tolerance=<n> [name=<c>] [structure=<c>]
```

Smooth a boundary structure:

```
filter_structure type=smooth \
    [factor=<n>] [mean_spacing=<n>] [name=<c>] [structure=<c>]
```

Note:

The `filter_structure` command with `type=smooth` is not available for 2D structures.

Create a boundary structure from a PMC structure (see [Saving Boundaries for PMC Structures on page 538](#)):

```
filter_structure type=vbe [decimate=<b> [accuracy=<n>]] \
    [grain_regions=<b>] [include_grain_index=<b>] \
    [material_priority=<l>] [material_selection=<c>] [structure=<c>]
```

Note:

When you start Sentaurus Topography 3D with the `--processes` command-line option with a value greater than 1 (see [Table 1 on page 18](#)), except when `type=copy`, the parameter `structure` must not denote a structure obtained from the `etch` command using `method=pmc averaging_runs=1`.

Chapter 6: Input Commands

filter_structure

Table 69 Parameters of filter_structure command

Parameter	Description
accuracy	<p>Sets the maximum deformation during decimation of the boundary structure as follows:</p> <ul style="list-style-type: none"> When <code>type=rediscretize_boundary</code> and <code>method</code> is not set to <code>dc</code>, the <code>accuracy</code> parameter specifies the maximum deformation during the decimation of the rediscretized boundary relative to the value of the <code>mean_spacing</code> parameter. When <code>type=vbe</code>, the <code>accuracy</code> parameter specifies the maximum deformation during the decimation of the boundary extracted with the volume boundary extraction (VBE) method relative to the mean PMC spacing. <p>It can be specified only if <code>decimate=true</code>.</p> <p>Type: Number Default: <code>1e-3</code> Range: $[0, \infty[$</p>
body	<p>Sets the name of the structure to use as the body of the Boolean operation. If omitted, the structure specified with the parameter <code>structure</code> will be used as the body.</p> <p>Type: Character Default: none</p>
boolean_accuracy	<p>Sets the maximum deviation between the decimated surface of the boundary structure produced by Boolean operations and its original surface.</p> <p>When set to <code>-1</code>, the used value is half of the structure-dependent spacing <code>epsilon</code>¹.</p> <p>It can be specified only if <code>decimate=true</code>.</p> <p>Type: Number Default: <code>-1</code> Range: $\{-1\} \cup [0, \infty[$ Unit: μm</p>
dc_min_angle	<p>When <code>type=dc</code> or <code>type=rediscretize_boundary</code> and <code>method=dc</code>, this parameter sets the minimum angle of the surface mesh.</p> <p>Type: Number Default: Value of <code>dc_min_angle</code> parameter of <code>let</code> command Range: $[0, 180]$ Unit: degree</p>

Chapter 6: Input Commands

filter_structure

Table 69 Parameters of filter_structure command (Continued)

Parameter	Description
dc_min_dihedral_angle	When <code>type=dc</code> or <code>type=rediscretize_boundary</code> and <code>method=dc</code> , this parameter sets the minimum dihedral angle of the surface mesh. Type: Number Default: Value of <code>dc_min_dihedral_angle</code> parameter of <code>let</code> command Range: [0, 180] Unit: degree
dc_reference_volume_scaling	When <code>type=dc</code> , this parameter allows you to adjust the surface location when converting a PMC structure to a boundary. Larger values expand the structure into the gas. Type: Number Default: none Range:]0, 2[Unit: unitless
dc_snap_to_box	When <code>type=dc</code> and <code>dc_snap_to_box=true</code> , this parameter snaps the outer boundary points to the bounding box. This can help tools that read the boundary to create a bulk mesh. Type: Boolean Default: true
dc_version	Selects the version of the dual-contouring algorithm. Options are: <ul style="list-style-type: none"> • 1: Selects the algorithm available in releases prior to S-2021.06. • 2: Selects the algorithm available starting from S-2021.06. Type: Number Default: 1
decimate	Specifies whether to decimate the boundary structure as follows: <ul style="list-style-type: none"> • When <code>type=boolean</code>, decimation is produced by Boolean operations. • When <code>type=rediscretize_boundary</code> and <code>method</code> is not set to <code>dc</code>, decimation is specified by the <code>structure</code> parameter. • When <code>type=vbe</code>, decimation uses the VBE method. Type: Boolean Default: true

Chapter 6: Input Commands

filter_structure

Table 69 Parameters of *filter_structure* command (Continued)

Parameter	Description
deposit_material	<p>Sets the material to assign to all the deposited regions of a structure obtained from a PMC simulation when executing Boolean operations as follows:</p> <ul style="list-style-type: none">• When processing the result of a PMC simulation where a single material was deposited and <code>deposit_material</code> was not specified, that material is used as the deposited material for Boolean operations.• If multiple materials were deposited in a PMC simulation, then <code>Anymaterial</code> is used as the deposited material for Boolean operations if <code>deposit_material</code> was not specified.• If <code>deposit_material</code> is specified, that material is used as the deposited material for Boolean operations. <p>Type: Character Default: See Description</p>
exposed_only	<p>Specifies whether only exposed parts should be removed. This parameter applies only to boundary structures.</p> <p>Type: Boolean Default: true</p>
factor	<p>Sets how strong the smoothing is relative to the mean spacing of the last preceding etching or deposition step. Higher values cause stronger smoothing.</p> <p>Type: Number Default: 1 Range: [0.2, 5]</p>
grain_regions	<p>Specifies whether the boundary structure produced by the VBE method should contain different regions for portions of the structure with the same material but with different material properties.</p> <p>Note: The VBE method can create boundary structures with no more than 240 regions.</p> <p>Type: Boolean Default: false</p>

Chapter 6: Input Commands

filter_structure

Table 69 Parameters of filter_structure command (Continued)

Parameter	Description
include_grain_index	<p>Specifies whether to store the material property (grain index in polycrystalline materials) as a field when converting PMC to brep structures using the VBE or DC method.</p> <p>If <code>include_grain_index=true</code>, then when converting from PMC to boundary format, the command writes the grain index as a field into the structure for the <code>filter_structure</code> command, or directly to the file for the <code>save</code> command.</p> <p>Best results are obtained using the <code>filter_structure</code> command with <code>decimate=false</code> to create a boundary with a fine mesh for viewing the field.</p> <p>Type: Boolean Default: false</p>
keep_top_gas	<p>Specifies whether to keep the top gas. This parameter applies only to the dual-contouring method (<code>type=dc</code>).</p> <p>Type: Boolean Default: false</p>
material	<p>Sets the material to replace. At least one region with the specified material must exist.</p> <p>Type: Character Default: none</p>
material_priority	<p>Sets a material priority list for materials at interfaces when using the VBE method.</p> <p>Type: List Default: none</p>
material_selection	<p>Sets the algorithm used to select the materials of a PMC cell when using the VBE method (see Saving Boundaries for PMC Structures on page 538). Options are:</p> <ul style="list-style-type: none"> • maximum • mixed • proportional <p>Type: Character Default: mixed</p>
materials	<p>Sets the materials of the parts to remove. If omitted, a part will be removed if it matches the other specified criteria, independently of its material.</p> <p>Type: List Default: none</p>

Chapter 6: Input Commands

filter_structure

Table 69 Parameters of filter_structure command (Continued)

Parameter	Description
materials_in_contact	A part can be removed if all materials with which it is in contact are included in the list of materials specified by this parameter. If you omit this parameter, a part will be removed if it matches the other specified criteria. This parameter applies only to boundary structures. Type: List Default: none
maximum_area	Sets the maximum area of the parts to remove. If omitted, a part will be removed if it matches the other specified criteria, independently of its area. This parameter applies only to boundary structures. Type: Number Default: none Range: [0, ∞[Unit: μm^2
maximum_volume	Sets the maximum volume of the parts to remove. If omitted, a part will be removed if it matches the other specified criteria, independently of its volume. This parameter is mandatory when processing PMC structures. Type: Number Default: none Range: [0, ∞[Unit: μm^3
mean_spacing	Sets the mean spacing relative to which the decimation or smoothing is specified. Type: Number Default: Mean spacing of the last preceding etching or deposition step Range: [0, ∞[Unit: μm
merge_replacements	Specifies a list of material replacement maps defined in the define_material_replacement command. The list consists of the names of material replacement maps. PMC cells that contain the species matching the material replacement species and volume_fractions (with tolerance specified by merge_tolerance) are converted to the material specified by the material replacement map. Note: This parameter can be used only with PMC structures. Type: List Default: none

Chapter 6: Input Commands

filter_structure

Table 69 Parameters of filter_structure command (Continued)

Parameter	Description
merge_tolerance	Sets the allowed deviation from volume_fractions of the material replacement map, so as to perform the merge. Type: Number Default: 0.1
merged_regions	Sets the names of regions to be merged. Type: List Default: none
method	When type=rediscretize_boundary, this parameter sets the rediscretization method. Options are: <ul style="list-style-type: none">• dc: Dual-contouring method• vbe: VBE method Type: Character Default: none
min_angle	Sets the smallest angle in the elements of the surface of the boundary structure obtained by decimating as follows: <ul style="list-style-type: none">• When type=boolean, the boundary structure is produced by Boolean operations.• When type=decimate, the structure parameter specifies the boundary structure.• When type=rediscretize_boundary and method is not set to dc, the structure is a rediscretized boundary structure.• When type=vbe, the boundary structure is extracted using the VBE method. When type=rediscretize_boundary and when type=vbe, you can specify the min_angle parameter only if decimate=true. Type: Number Default: 0 Range: [0, 180] Unit: degree

Chapter 6: Input Commands

filter_structure

Table 69 Parameters of filter_structure command (Continued)

Parameter	Description
min_dihedral_angle	<p>Sets the smallest dihedral angle between two elements, which share an edge, in the surface of the boundary structure obtained by decimating as follows:</p> <ul style="list-style-type: none"> When <code>type=boolean</code>, the boundary structure is produced by Boolean operations. When <code>type=decimate</code>, the <code>structure</code> parameter specifies the boundary structure. When <code>type=rediscretize_boundary</code> and <code>method</code> is not set to <code>dc</code>, the structure is a rediscretized boundary structure. When <code>type=vbe</code>, the boundary structure is extracted using the VBE method. <p>When <code>type=rediscretize_boundary</code> and when <code>type=vbe</code>, you can specify the parameter <code>min_dihedral_angle</code> only if <code>decimate=true</code>.</p> <p>Type: Number Default: 0 Range: [0, 180] Unit: degree</p>
name	<p>Sets the name of the result structure. If omitted, the input structure will be replaced.</p> <p>Type: Character Default: none</p>
new_material	<p>Sets the name of the replacement material.</p> <p>Type: Character Default: none</p>
new_region_name	<p>When renaming regions, this parameter sets the new name for a region. No region with this name must exist before the renaming. When merging regions, this parameter specifies the name of the region created by merging. No region with this name must exist before the merge.</p> <p>Type: Character Default: none</p>
point_max	<p>Sets the maximum bounding vertex of the cuboid to which the parts to remove belong. If omitted, a part will be removed if it matches the other specified criteria, independently of its position. This parameter applies only to boundary structures.</p> <p>Type: Vector Default: none Unit: μm</p>

Chapter 6: Input Commands

filter_structure

Table 69 Parameters of filter_structure command (Continued)

Parameter	Description
point_min	<p>Sets the minimum bounding vertex of the cuboid to which the parts to remove belong. If omitted, a part will be removed if it matches the other specified criteria, independently of its position. This parameter applies only to boundary structures.</p> <p>Type: Vector Default: none Unit: μm</p>
region	<p>Sets the name of a region to remove or for which region the material will be replaced, or the name of a region to be renamed. The specified region must exist and, when removing a region, this region must not be the only region of the structure.</p> <p>Type: Character Default: none</p>
ridge_angle	<p>Sets the angle used to determine geometric features of the boundary structure obtained by decimating as follows:</p> <ul style="list-style-type: none"> When <code>type=boolean</code>, the boundary structure is produced by Boolean operations. When <code>type=decimate</code>, the <code>structure</code> parameter specifies the boundary structure. When <code>type=rediscretize_boundary</code> and <code>method</code> is not set to <code>dc</code>, the structure is a rediscretized boundary structure. When <code>type=vbe</code>, the boundary structure is extracted using the VBE method. <p>When <code>type=rediscretize_boundary</code> and when <code>type=vbe</code>, you can specify the <code>ridge_angle</code> parameter only if <code>decimate=true</code>.</p> <p>Type: Number Default: 179 Range: [0, 180] Unit: degree</p>

Chapter 6: Input Commands

filter_structure

Table 69 Parameters of filter_structure command (Continued)

Parameter	Description
shortest_edge	<p>Sets the shortest edge of the surface of the boundary structure obtained by decimation as follows:</p> <ul style="list-style-type: none"> • When <code>type=boolean</code>, decimates the boundary structure produced by Boolean operations. • When <code>type=decimate</code>, decimates the structure specified by the <code>structure</code> parameter. • When <code>type=rediscretize_boundary</code> and <code>method</code> is not set to <code>dc</code>, decimates the rediscretized boundary structure. • When <code>type=vbe</code>, decimates the boundary structure extracted using the VBE method. <p>When <code>type=rediscretize_boundary</code> and when <code>type=vbe</code>, you can specify the <code>shortest_edge</code> parameter only if <code>decimate=true</code>.</p> <p>Type: Number Default: <code>boolean_accuracy</code> (when <code>type=boolean</code>) <code>mean_spacing * tolerance</code> (when <code>type=decimate</code>) <code>mean_spacing * tolerance</code> (when <code>type=rediscretize_boundary</code> and <code>type=vbe</code>) Range: $[0, \infty[$ Unit: μm</p>
silent	<p>Specifies whether to write information about the parts being removed to the log file.</p> <p>Type: Boolean Default: <code>false</code></p>
spacing	<p>Sets the spacing to use to create a PMC structure. This parameter is mandatory if there is no preceding etching or deposition step specifying a spacing.</p> <p>Type: Number Default: Minimum spacing of the last preceding etching or deposition step Range: $]0, \infty[$ Unit: μm</p>

Chapter 6: Input Commands

filter_structure

Table 69 Parameters of filter_structure command (Continued)

Parameter	Description
split_replacements	<p>Specifies a list of material replacement maps defined in the <code>define_material_replacement</code> command. The list consists of the names of material replacement maps. The material is replaced by a list of species defined by the material replacement map before the PMC step begins.</p> <p>Note: This parameter can be used only with <code>method=pmc</code>.</p> <p>Type: List Default: none</p>
structure	<p>Sets the name of the structure that must be used for the Boolean operations (when <code>type=boolean</code>), or copied (when <code>type=copy</code>), or decimated (when <code>type=decimate</code>), or smoothed (when <code>type=smooth</code>), or from which the disconnected parts must be removed (when <code>type=remove_disconnected_top_parts</code>).</p> <p>Type: Character Default: default_structure</p>
surface_accuracy	<p>Sets the maximum deviation between the decimated exposed surface used as an operand of the Boolean operations and the original exposed surface.</p> <p>When set to -1, the used value is half of the structure-dependent spacing epsilon¹.</p> <p>It can be specified only if <code>surface_decimate=true</code>.</p> <p>Type: Number Default: -1 Range: {-1} ∪ [0, ∞[Unit: μm</p>
surface_decimate	<p>Specifies whether to decimate the exposed surface used as an operand of the Boolean operations.</p> <p>Type: Boolean Default: false</p>

Chapter 6: Input Commands

filter_structure

Table 69 Parameters of filter_structure command (Continued)

Parameter	Description
surface_min_angle	<p>Sets the smallest angle in the elements of the decimated exposed surface used as an operand of the Boolean operations.</p> <p>It can be specified only if <code>surface_decimate=true</code>.</p> <p>Type: Number Default: 0 Range: [0, 180] Unit: degree</p>
surface_min_dihedral_angle	<p>Sets the smallest dihedral angle between two elements, which share an edge, of the decimated exposed surface used as an operand of the Boolean operations.</p> <p>It can be specified only if <code>surface_decimate=true</code>.</p> <p>Type: Number Default: 0 Range: [0, 180] Unit: degree</p>
surface_ridge_angle	<p>Sets the angle used by the decimation algorithm to determine geometric features of the exposed surface used as an operand of the Boolean operations.</p> <p>It can be specified only if <code>surface_decimate=true</code>.</p> <p>Type: Number Default: 179 Range: [0, 180] Unit: degree</p>
surface_shortest_edge	<p>Sets the shortest edge of the decimated exposed surface used as an operand of the Boolean operations.</p> <p>When set to -1, the used value is half of the structure-dependent spacing epsilon¹.</p> <p>It can be specified only if <code>surface_decimate=true</code>.</p> <p>Type: Number Default: -1 Range: {-1} \cup [0, ∞[Unit: μm</p>

Chapter 6: Input Commands

filter_structure

Table 69 Parameters of filter_structure command (Continued)

Parameter	Description
surface_simplify	<p>Specifies whether the exposed surface of a structure obtained from a PMC simulation should be decimated before executing Boolean operations.</p> <p>Note: This parameter is deprecated. Use <code>surface_decimate</code> instead.</p> <p>Type: Boolean Default: false</p>
tolerance	<p>Sets the tolerance relative to the mean spacing for decimating the number of surface elements. Higher values cause stronger decimation.</p> <p>Type: Number Default: none Range: [0, 1]</p>
top_gas_thickness	<p>Sets the minimum thickness of the gas region added on top of the created PMC structure.</p> <p>Type: Number Default: 0 Range: [0, ∞[Unit: μm</p>
type	<p>Sets the type of operation. Table 70 lists the operation types and summarizes, for each value of <code>type</code>, which structure type it can operate on (the parameter <code>structure</code>) and the type of the result structure (the parameter <code>name</code>).</p> <p>Type: Character Default: none</p>

1. The structure-dependent spacing `epsilon` is logged out when defining a structure using the `define_structure` command.

Table 70 Supported input structures for different values of type parameter

Type	Input structure		Output structure
	Boundary	PMC	
boolean	Not supported	Supported	Boundary
convert_to_pmc	Supported	Not supported	PMC

Chapter 6: Input Commands

filter_structure

Table 70 Supported input structures for different values of type parameter (Continued)

Type	Input structure		Output structure
	Boundary	PMC	
copy	Supported	Supported	Same type as input
dc	Not supported	Supported	Boundary
decimate	Supported	Not supported	Boundary
merge_regions	Supported	Not supported	Boundary
rediscretize_boundary	Supported	Not supported	Boundary
remove_damage	Not supported	Supported	PMC
remove_disconnected_top_parts	Supported	Not supported	Boundary
remove_parts	Supported	Supported	Same type as input
remove_region	Supported	Not supported	Boundary
rename_region	Supported	Not supported	Boundary
replace_material	Supported	Not supported	Boundary
smooth	Supported	Not supported	Boundary
vbe	Not supported	Supported	Boundary

Description

The default value of the mean spacing is calculated from the last preceding `etch` or `deposit` command. If there is no such command, the mean spacing must be specified with the parameter `mean_spacing`.

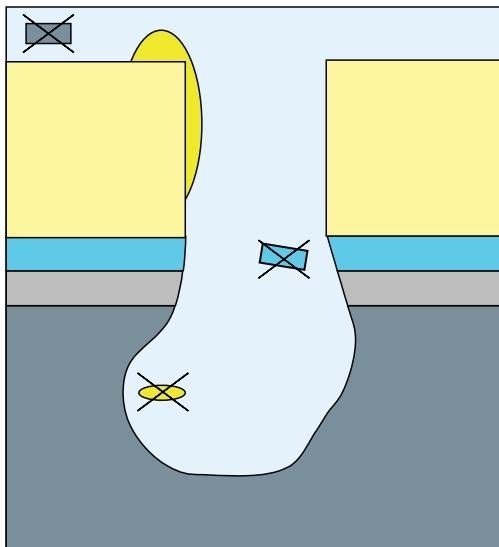
The default value of the spacing parameter is calculated from the last preceding `etch` or `deposit` command specifying a spacing. If there is no such command, the spacing must be specified with the parameter `spacing`.

Creating a boundary structure from a PMC structure is very similar to saving a boundary structure from a PMC structure except that a new structure is created instead of saving it to a TDR file. For more information about the VBE method, see [Saving Boundaries for PMC Structures on page 538](#).

Chapter 6: Input Commands

finalize_model

Figure 34 Using the filter_structure type=remove_disconnected_top_parts command removes the three cross-out parts



finalize_model

This command is used to indicate that the definition of the specified model is completed.

Following this command, the specified model cannot be modified using the command add_float_parameter, add_formula, add_int_parameter, add_reaction, or add_source_species.

Before using the command add_flux_properties, add_reaction_properties, define_deposit_machine, or define_etch_machine for the specified model, you must specify the finalize_model command.

Syntax

```
finalize_model model=<c>
```

Table 71 Parameters of finalize_model command

Parameter	Description
model	Sets the name of the model that is finalized. Type: Character Default: none

layout

This command queries the properties of a layout that has been created with the `define_layout` command (see [define_layout on page 278](#)).

Syntax

Query the bounding box of the specified 3D domain:

```
layout domain=<c> name=<c> type=bounding_box [silent=<b>]
```

Query the names of 3D domains defined in a layout:

```
layout name=<c> type=domains [silent=<b>]
```

Query the names of layers defined in a layout:

```
layout name=<c> type=layers [silent=<b>]
```

Table 72 Parameters of layout command

Parameter	Description
domain	Sets the name of the domain for which the bounding box is queried. Type: Character Default: none
name	Sets the name of the layout. Type: Character Default: default_layout
silent	Specifies how the query results are returned. Options are: <ul style="list-style-type: none">When <code>silent=false</code>, the results are returned as a Tcl list and are written to the log file.When <code>silent=true</code>, the results are returned as a Tcl list but are not written to the log file. Type: Boolean Default: false
type	Sets the type of the query. Options are: <ul style="list-style-type: none"><code>bounding_box</code><code>domains</code><code>layers</code> Type: Character Default: none

Chapter 6: Input Commands

let

let

This command sets the global properties of Sentaurus Topography 3D, one parameter at a time.

Syntax

```
let <parameter>=<type>
```

Table 73 Parameters of let command

Parameter	Description
base_name	<p>Sets the base name of output files (see Output Files on page 20).</p> <p>Note: When Sentaurus Topography 3D is given the command file <code>commandfile.extension</code>, the command <code>let base_name=commandfile</code> is executed before starting to process the given command file.</p> <p>Type: Character Default: none</p>
compatibility_version	<p>Sets the version of Sentaurus Topography 3D with which the results must be compatible. Options are:</p> <ul style="list-style-type: none">• U-2022.12• T-2022.03• S-2021.06• R-2020.09• Q-2019.12• P-2019.03• O-2018.06• N-2017.09 <p>Type: Character Default: U-2022.12</p>
dc_keep_top_gas	<p>Specifies whether to keep the top gas when the dual-contouring method is used to convert a PMC structure to a boundary structure because <code>pmc_to_brep_conversion_method=dc</code> is specified.</p> <p>Type: Boolean Default: false</p>

Table 73 Parameters of let command (Continued)

Parameter	Description
dc_min_angle	<p>Sets the minimum angle of the surface mesh for the dual-contouring method (see Dual-Contouring Method on page 539) in the following cases:</p> <ul style="list-style-type: none"> The dual-contouring method is used to convert a PMC structure to a boundary structure because <code>dc_version_for_pmc_to_brep_conversion=dc</code> is specified In the command <code>filter_structure type=dc</code> when its <code>dc_min_angle</code> parameter is not specified In the command <code>save type=dc</code> when its <code>dc_min_angle</code> parameter is not specified <p>Type: Number Default: <code>1e-6</code> Range: <code>[0, 180]</code> Unit: degree</p>
dc_min_dihedral_angle	<p>Sets the minimum dihedral angle of the surface mesh for the dual-contouring method (see Dual-Contouring Method on page 539) in the following cases:</p> <ul style="list-style-type: none"> The dual-contouring method is used to convert a PMC structure to a boundary structure because <code>dc_version_for_pmc_to_brep_conversion=dc</code> is specified In the command <code>filter_structure type=dc</code> when its parameter <code>dc_min_dihedral_angle</code> is not specified In the command <code>save type=dc</code> when its parameter <code>dc_min_dihedral_angle</code> is not specified <p>Type: Number Default: <code>5e-6</code> Range: <code>[0, 180]</code> Unit: degree</p>
dc_snap_to_box	<p>Specifies whether to snap the outer boundary points to the bounding box when the dual-contouring method is used to convert a PMC structure to a boundary structure because <code>dc_version_for_pmc_to_brep_conversion=dc</code> is specified. This can help tools that read the boundary to create a bulk mesh.</p> <p>Type: Boolean Default: <code>true</code></p>

Chapter 6: Input Commands

let

Table 73 Parameters of let command (Continued)

Parameter	Description
dc_version_for_pmc_slicing	Selects the version of the dual-contouring algorithm for extract slicing during PMC steps. Options are: <ul style="list-style-type: none">• 1: Selects the algorithm available in releases prior to S-2021.06.• 2: Selects the algorithm available starting from S-2021.06. Type: Number Default: 1
dc_version_for_pmc_to_brep_conversion	Selects the version of the dual-contouring algorithm. Options are: <ul style="list-style-type: none">• 1: Selects the algorithm available in releases prior to S-2021.06.• 2: Selects the algorithm available starting from S-2021.06. Type: Number Default: 1
decimate	Specifies whether to decimate boundary structures. Type: Boolean Default: true
decimate_accuracy	Sets the maximum deviation between the decimated surface of a boundary structure and its original surface. When set to -1, the used value is half of the structure-dependent spacing epsilon ¹ . Type: Number Default: -1 Range: {-1} \cup [0, ∞ [Unit: μm
decimate_min_angle	Sets the smallest angle in the elements of the surface of the boundary structure produced by the decimation algorithm. Type: Number Default: 0 Range: [0, 180] Unit: degree
decimate_min_dihedral_angle	Sets the smallest dihedral angle between two elements, which share an edge, of the surface of the boundary structure produced by the decimation algorithm. Type: Number Default: 0 Range: [0, 180] Unit: degree

Chapter 6: Input Commands

let

Table 73 Parameters of let command (Continued)

Parameter	Description
decimate_ridge_angle	<p>Sets the angle used by the decimation algorithm to determine the geometric features of a boundary structure.</p> <p>Type: Number Default: 179 Range: [0, 180] Unit: degree</p>
decimate_shortest_edge	<p>Sets the shortest edge of the surface of the boundary structure produced by the decimation algorithm.</p> <p>When set to -1, the used value is half of the structure-dependent spacing epsilon¹.</p> <p>Type: Number Default: -1 Range: {-1} ∪ [0, ∞[Unit: μm</p>
keep_parallel_licenses	<p>Specifies whether parallel licenses must remain checked out after a command using them has been executed.</p> <p>Note: This parameter has no effect if you specify the command-line option --keep_parallel_licenses when Sentaurus Topography 3D is started (see Table 1 on page 18).</p> <p>Type: Boolean Default: false</p>
log_file	<p>Sets the name of the log file.</p> <p>In the file name, <base_name> denotes the value of the base_name parameter of the let command.</p> <p>Type: Character Default: <base_name>.log</p>
log_level	<p>Sets the verbosity level. Options are:</p> <ul style="list-style-type: none"> • all: Saves all output to the log file. • error: Saves only error messages to the log file. • info: Saves minimal output to the log file. <p>Type: Character Default: info</p>

Chapter 6: Input Commands

let

Table 73 Parameters of let command (Continued)

Parameter	Description
log_target	<p>Sets the log output. Options are:</p> <ul style="list-style-type: none">• both: Directs output to the log file and screen.• console: Directs output only to the screen.• file: Directs output only to the log file. <p>Type: Character Default: both</p>
num_threads	<p>Sets the number of threads per process to be used to execute the commands that support shared-memory parallelization. Only valid if <code>let parallel=true</code>.</p> <p>If no value is specified, an implementation-defined optimum number of threads is used. See Advanced Shared-Memory Parallelization Options on page 42.</p> <p>Note: With regard to this parameter:</p> <ul style="list-style-type: none">• This parameter has no effect if you specify the command-line option <code>--threads</code> when Sentaurus Topography 3D is started (see Table 1 on page 18).• When running Sentaurus Topography 3D from Sentaurus Workbench using auto-detection of threads, an error is issued if no value is specified.• If the value for <code>num_threads</code> is larger than the one for the <code>--max_threads</code> command-line option, Sentaurus Topography 3D uses the value of <code>--max_threads</code>. <p>Type: Number Default: Automatic Range: [1...256]</p>
parallel	<p>Specifies whether to activate parallel computation for models that support parallel computation (see Basic Shared-Memory Parallelization on page 41).</p> <p>Note: This parameter has no effect if you specify the command-line option <code>--threads</code> when Sentaurus Topography 3D is started (see Table 1 on page 18).</p> <p>Type: Boolean Default: false</p>

Chapter 6: Input Commands

let

Table 73 Parameters of let command (Continued)

Parameter	Description
parallel_license	<p>Sets the behavior of the simulator if the number of requested threads cannot be used due to a lack of the respective number of parallel licenses (see Advanced Shared-Memory Parallelization Options on page 42). Options are:</p> <ul style="list-style-type: none">• abort: Terminates the simulation.• available: Checks out the maximum number of available licenses, and uses the maximum number of threads available. If commands are parallelized using MPI, this option terminates the simulation if the maximum number of available threads is less than the number of requested processes.• serial: If commands are not parallelized using MPI, this option continues the simulation in serial mode. If commands are parallelized using MPI, this option terminates the simulation.• wait: Waits until enough parallel licenses become available. <p>Type: Character Default: serial</p>
pmc_bca_sra	<p>Specifies whether to apply a more accurate material determination during cascade computation, and when finding ion material collisions.</p> <p>Type: Boolean Default: false</p>
pmc_boolean_correction	<p>If let pmc_to_brep_conversion_method=boolean, then this parameter specifies to apply a correction algorithm at every PMC step when updating the stored body structure.</p> <p>Type: Boolean Default: false</p>

Chapter 6: Input Commands

let

Table 73 Parameters of let command (Continued)

Parameter	Description
pmc_to_brep_conversion_method	<p>Sets the method to use to convert a PMC structure to a boundary structure whenever a boundary structure is expected, but a PMC structure is given. Options are:</p> <ul style="list-style-type: none"> • boolean • dc • error • vbe <p>Note:</p> <p>When <code>error</code> is specified, an error message is issued whenever a boundary structure is expected, but a PMC structure is given.</p> <p>When <code>boolean</code> is specified, the body structure is stored in the PMC structure and is updated automatically at every step, obviating the need for <code>filter_structure type=boolean</code> commands.</p> <p>Type: Character Default: <code>vbe</code></p>
snmesh_repair	<p>Specifies whether to repair the structure after Boolean operations. Activating repair reduces very thin regions and facilitates meshing of the structure.</p> <p>Note:</p> <p>The repair functionality sometimes uses excessive CPU time and memory.</p> <p>Type: Boolean Default: <code>false</code></p>
surface_decimate	<p>Specifies whether to decimate the exposed surface.</p> <p>Type: Boolean Default: <code>true</code></p>
surface_decimate_accuracy	<p>Sets the maximum deviation between the decimated exposed surface and the original exposed surface.</p> <p>When set to <code>-1</code>, the used value is half of the structure-dependent spacing epsilon¹.</p> <p>Type: Number Default: <code>-1</code> Range: $\{-1\} \cup [0, \infty[$ Unit: μm</p>

Chapter 6: Input Commands

let

Table 73 Parameters of let command (Continued)

Parameter	Description
surface_decimate_min_angle	Sets the smallest angle in the elements of the exposed surface produced by the decimation algorithm. Type: Number Default: 0 Range: [0, 180] Unit: degree
surface_decimate_min_dihedral_angle	Sets the smallest dihedral angle between two elements, which share an edge, of the exposed surface produced by the decimation algorithm. Type: Number Default: 0 Range: [0, 180] Unit: degree
surface_decimate_ridge_angle	Sets the angle used by the decimation algorithm to determine geometric features of the exposed surface. Type: Number Default: 179 Range: [0, 180] Unit: degree
surface_decimate_shortest_edge	Sets the shortest edge of the decimated exposed surface. When set to -1, the used value is half of the structure-dependent spacing epsilon ¹ . Type: Number Default: -1 Range: {-1} ∪ [0, ∞[Unit: μm
vbe_material_priority	Sets a material priority list for materials at interfaces when the VBE method is used to convert a PMC structure to a boundary structure because <code>pmc_to_brep_conversion_method=vbe</code> is specified. Type: List Default: none

Chapter 6: Input Commands

let

Table 73 Parameters of let command (Continued)

Parameter	Description
vbe_material_selection	Sets the algorithm used to select the materials mixed in a PMC cell when the VBE method is used to convert a PMC structure to a boundary structure because <code>pmc_to_brep_conversion_method=vbe</code> is specified (see Volume Boundary Extraction Method on page 539). Options are: <ul style="list-style-type: none">• maximum• mixed• proportional Type: Character Default: mixed

1. *The structure-dependent spacing epsilon is logged out when defining a structure using the `define_structure` command.*

Examples

Set the verbosity level to error messages only, direct the output to both the screen and log file, and set a name for the log file:

```
let log_level=error
let log_target=both
let log_file=out.log
```

Activate parallel computation and set the number of threads:

```
let parallel=true
let num_threads=8
```

litho

This command performs a lithography simulation and adds a resist region.

Note:

The `litho` command is not available for 2D structures.

When you start Sentaurus Topography 3D with the `--processes` command-line option with a value greater than 1 (see [Table 1 on page 18](#)), the parameter `structure` must not denote a structure obtained from the `etch` command using `method=pmc averaging_runs=1`.

Syntax

```
litho inputfile=<c> \
    [accuracy=<n>] [comment=<c>] [decimate=<b>] [machine=<c>] \
    [mask=<c>] [material=<c>] [min_angle=<n>] \
    [min_dihedral_angle=<n>] \
    [merge=<b>] [options=<c>] [outputfile=<c>] [region=<c>] \
    [ridge_angle=<n>] [shortest_edge=<n>] [structure=<c>]
```

Table 74 Parameters of `litho` command

Parameter	Description
accuracy	<p>Sets the maximum deviation between the decimated surface of the boundary structure produced by Boolean operations and its original surface.</p> <p>When set to <code>-1</code>, the used value is half of the structure-dependent spacing <code>epsilon</code>¹.</p> <p>It can be specified only if <code>decimate=true</code>, or if you do not specify the <code>decimate</code> parameter and specify <code>let decimate=true</code>.</p> <p>Type: Number Default: Value set by <code>let decimate_accuracy=<n></code> Range: $\{-1\} \cup [0, \infty[$ Unit: μm</p>
comment	<p>Sets a comment for this process step that will be displayed or written to the log file.</p> <p>Type: Character Default: empty string</p>

Chapter 6: Input Commands

litho

Table 74 Parameters of litho command (Continued)

Parameter	Description
decimate	Specifies whether to decimate the boundary structure produced by Boolean operations. Type: Boolean Default: Value set by <code>let decimate=</code>
inputfile	Sets the name of the input SLO file. Type: Character Default: none
machine	Sets the name of the lithography machine to be used. This must be predefined with the <code>define_litho_machine</code> command. Type: Character Default: default_machine
mask	Sets the name of the mask file to be used. Note: If this parameter is not specified, the mask specified in the SLO file is used for the lithography simulation. Type: Character Default: none
material	Sets the name of the material of the created region. Type: Character Default: photoresist
merge	Specifies whether the deposited region merges with already existing regions of the same material in the structure. Type: Boolean Default: false
min_angle	Sets the smallest angle in the elements of the decimated surface of the boundary structure produced by Boolean operations. It can be specified only if <code>decimate=true</code> , or if you do not specify the <code>decimate</code> parameter and specify <code>let decimate=true</code> . Type: Number Default: Value set by <code>let decimate_min_angle=<n></code> Range: [0, 180] Unit: degree

Chapter 6: Input Commands

litho

Table 74 Parameters of litho command (Continued)

Parameter	Description
min_dihedral_angle	<p>Sets the smallest dihedral angle between two elements of the decimated surface of the boundary structure produced by Boolean operations that share an edge.</p> <p>It can be specified only if <code>decimate=true</code>, or if you do not specify the <code>decimate</code> parameter and specify <code>let decimate=true</code>.</p> <p>Type: Number Default: Value set by <code>let decimate_min_dihedral_angle=<n></code> Range: [0, 180] Unit: degree</p>
options	<p>Sets additional command-line options for Sentaurus Lithography.</p> <p>Note: If you specify more than one option, then they must be enclosed in double quotation marks.</p> <p>Type: Character Default: none</p>
outputfile	<p>Sets the name of the output SLO file.</p> <p>Type: Character Default: none</p>
region	<p>Sets the name of the resist region that is created.</p> <p>Type: Character Default: none</p>
ridge_angle	<p>Sets the angle used by the decimation algorithm to determine geometric features of the boundary structure produced by Boolean operations.</p> <p>It can be specified only if <code>decimate=true</code>, or if you do not specify the <code>decimate</code> parameter and specify <code>let decimate=true</code>.</p> <p>Type: Number Default: Value set by <code>let decimate_ridge_angle=<n></code> Range: [0, 180] Unit: degree</p>

Chapter 6: Input Commands

litho

Table 74 Parameters of *litho* command (Continued)

Parameter	Description
shortest_edge	<p>Sets the shortest edge of the decimated surface of the boundary structure produced by Boolean operations.</p> <p>When set to -1, the used value is half of the structure-dependent spacing epsilon¹.</p> <p>It can be specified only if <code>decimate=true</code>, or if you do not specify the <code>decimate</code> parameter and specify <code>let decimate=true</code>.</p> <p>Type: Number</p> <p>Default: Value set by <code>let decimate_shortest_edge=<n></code></p> <p>Range: $\{-1\} \cup [0, \infty[$</p> <p>Unit: μm</p>
structure	<p>Sets the name of the structure on which a lithography simulation must be run.</p> <p>Note:</p> <p>This parameter cannot specify a PMC structure. To process such a structure, an explicit conversion of the structure is needed before calling the <code>litho</code> command (see Integration With Other Sentaurus Topography 3D Functionality on page 580).</p> <p>Type: Character</p> <p>Default: <code>default_structure</code></p>

1. The structure-dependent spacing `epsilon` is logged out when defining a structure using the `define_structure` command.

pattern

This command uses logical masks defined with the `define_mask` command to create patterned profiles on top of an existing structure (see [define_mask on page 281](#)).

Note:

The `pattern` command is not available for 2D structures.

When you start Sentaurus Topography 3D with the `--processes` command-line option with a value greater than 1 (see [Table 1 on page 18](#)), the parameter `structure` must not denote a structure obtained from the `etch` command using `method=pmc averaging_runs=1`.

Syntax

Create a patterned profile on top of a boundary structure:

```
pattern material=<c> thickness=<n> type=<c> \
[accuracy=<n>] [comment=<c>] [decimate=<b>] [mask=<c>] \
[merge=<b>] [min_angle=<n>] [min_dihedral_angle=<n>] [region=<c>] \
[ridge_angle=<n>] [shortest_edge=<n>] [structure=<c>]
```

Create a patterned profile on top of a PMC structure:

```
pattern material=<c> thickness=<c> type=<c> \
[comment=<c>] [mask=<c>] [structure=<c>]
```

Table 75 Parameters of pattern command

Parameter	Description
accuracy	<p>Sets the maximum deviation between the decimated surface of the boundary structure produced by Boolean operations and its original surface.</p> <p>When set to -1, the used value is half of the structure-dependent spacing <code>epsilon</code>¹.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none">• The <code>structure</code> parameter denotes a boundary structure.• You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_accuracy=<n></code> Range: $\{-1\} \cup [0, \infty[$ Unit: μm</p>

Chapter 6: Input Commands

pattern

Table 75 Parameters of pattern command (Continued)

Parameter	Description
comment	Sets a comment for this process step that will be displayed or written to the log file. Type: Character Default: empty string
decimate	Specifies whether to decimate the boundary structure produced by Boolean operations. It can be specified only if <code>structure</code> denotes a boundary structure. Type: Boolean Default: Value set by <code>let decimate=</code>
mask	Sets the name of the mask defined in a <code>define_mask</code> command. Type: Character Default: <code>default_mask</code>
material	Sets the material of the pattern that is deposited on the structure. Type: Character Default: none
merge	Specifies whether the deposited region merges with already existing regions of the same material in the structure. It can be specified only if <code>structure</code> denotes a boundary structure. Type: Boolean Default: false
min_angle	Sets the smallest angle in the elements of the decimated surface of the boundary structure produced by Boolean operations. This parameter can be specified only if all of the following conditions are met: <ul style="list-style-type: none"> The <code>structure</code> parameter denotes a boundary structure. You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. Type: Number Default: Value set by <code>let decimate_min_angle=<n></code> Range: [0, 180] Unit: degree

Chapter 6: Input Commands

pattern

Table 75 Parameters of pattern command (Continued)

Parameter	Description
min_dihedral_angle	<p>Sets the smallest dihedral angle between two elements of the decimated surface of the boundary structure produced by Boolean operations that share an edge.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none"> • The <code>structure</code> parameter denotes a boundary structure. • You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_min_dihedral_angle=<n></code> Range: [0, 180] Unit: degree</p>
region	<p>Sets the region name of the pattern that is created. It can be specified only if <code>structure</code> denotes a boundary structure.</p> <p>Type: Character Default: none</p>
ridge_angle	<p>Sets the angle used by the decimation algorithm to determine geometric features of the boundary structure produced by Boolean operations.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none"> • The <code>structure</code> parameter denotes a boundary structure. • You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_ridge_angle=<n></code> Range: [0, 180] Unit: degree</p>

Chapter 6: Input Commands

pattern

Table 75 Parameters of pattern command (Continued)

Parameter	Description
shortest_edge	<p>Sets the shortest edge of the decimated surface of the boundary structure produced by Boolean operations.</p> <p>When set to -1, the used value is half of the structure-dependent spacing epsilon¹.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none"> • The <code>structure</code> parameter denotes a boundary structure. • You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_shortest_edge=<n></code> Range: {-1} \cup [0, ∞[Unit: μm</p>
structure	<p>Sets the name of the structure that must be patterned.</p> <p>Note: This parameter cannot specify a PMC structure. To process such a structure, an explicit conversion of the structure is needed before calling the <code>pattern</code> command (see Integration With Other Sentaurus Topography 3D Functionality on page 580).</p> <p>Type: Character Default: <code>default_structure</code></p>
thickness	<p>Sets the thickness of the pattern, measured from the top of the structure.</p> <p>Type: Number Default: none Range: [0, ∞[Unit: μm</p>
type	<p>Sets the type of the reticle and the resist. Options are:</p> <ul style="list-style-type: none"> • <code>dark_negative</code> • <code>dark_positive</code> • <code>light_negative</code> • <code>light_positive</code> <p>Type: Character Default: none</p>

1. The structure-dependent spacing `epsilon` is logged out when defining a structure using the `define_structure` command.

Description

The `pattern` command provides a convenient way to deposit a new region that depends on a logical mask by combining several process steps.

Depending on the type of the deposited material, there are different ways to interpret the `pattern` command:

- When creating a resist region, the `pattern` command can be interpreted as a shortcut for the following process steps:
 - Deposition of a negative or positive resist
 - Exposure of the resist with a dark-field or a light-field reticle
 - Development of the resist
- When creating a region with a different material, the `pattern` command can be interpreted as a shortcut for the following process steps:
 - Deposition of the material
 - Deposition of a negative or positive resist
 - Exposure of the resist with a dark-field or a light-field reticle
 - Development of the resist
 - Geometric etching of the deposited material
 - Stripping of the resist

A reticle is a physical representation of a logical mask that has been created from a layout layer or by operations on one or more logical masks. A reticle has one of two types depending on whether the mask areas covered by polygons transmit or block light:

- When exposing a reticle of type *dark field*, light is transmitted in areas that lie inside of the layout polygons, and light is blocked in areas that lie outside of the layout polygons.
- When exposing a reticle of type *light field*, light is transmitted in areas that lie outside of the layout polygons, and light is blocked in areas that lie inside of the layout polygons.

Similar to a reticle, there are different types of resist:

- When exposed and developed, a negative resist is removed from areas that were not exposed to light, and it remains in areas that were exposed to light.
- When exposed and developed, a positive resist is removed from areas that were exposed to light, and it remains in areas that were not exposed to light.

Chapter 6: Input Commands

pattern

There are different combinations of reticle and resist types, but there are only two possibilities for how material is deposited, as follows:

- Material is deposited in areas where the polygons are located in the logical mask (`dark_negative` and `light_positive`).
- Material is deposited in areas that are not covered by polygons in the logical mask (`dark_positive` and `light_negative`).

When only looking at the resulting region, it is redundant to provide all four combinations. However, providing all four combinations makes it possible to specify the intended type of processing explicitly.

Examples

This command uses `default_mask` to pattern a film consisting of silicon material, with a thickness of 0.1 µm, measured from the top of the current structure:

```
pattern material=Silicon thickness=0.1
```

Example using a mask and a region name:

```
pattern material=Silicon thickness=0.1 mask=mask_1 \
comment="pattern mask 1" region=mask_1_pattern
```

This command uses the mask `mask_1` to pattern a film consisting of silicon material, with a thickness of 0.1 µm, measured from the top of the device. The patterned region is given the name `mask_1_pattern`.

The comment for the process step is “pattern mask 1” and is displayed in the log file.

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remove_material

remove_material

This command removes material from a boundary structure or PMC structure.

Syntax

```
remove_material material=<c> [comment=<c>] [exposed_only=<b>] \
[structure=<c>]
```

Table 76 Parameters of remove_material command

Parameter	Description
comment	Sets a comment for this process step that will be displayed or written to the log file. Type: Character Default: empty string
exposed_only	Specifies whether only the exposed material must be removed or all materials. Type: Boolean Default: true
material	Sets the material to be removed from the structure. Type: Character Default: none
structure	Sets the name of the structure from which a material must be removed. Type: Character Default: default_structure

Examples

Remove all of the exposed silicon material from the structure (silicon that is completely covered by other material is not removed):

```
remove_material material=Silicon comment="strip silicon"
```

Chapter 6: Input Commands

save

save

This command saves or extracts different structures as well as pattern density-related functions, NADs, IADs, species distributions, probabilities, reflection, and yield functions.

Syntax

Save a boundary structure to a TDR file:

```
save type=final_structure [add_interfaces=<b>] [file=<c>] \
[force_save=<b>] [structure=<c>] [tdr_geometry=<c>]
```

Extract the exposed surface of a boundary structure and save it to a TDR file:

```
save type=exposed_surface [file=<c>] [force_save=<b>] \
[include_disconnected_parts=<b>] [include_voids=<b>] \
[structure=<c>] [tdr_geometry=<c>]
```

Extract the closed exposed surface of a boundary structure and save it to a TDR file:

```
save type=closed_surface [file=<c>] [force_save=<b>] \
[structure=<c>] [tdr_geometry=<c>]
```

Save a PMC structure converted to a boundary structure using the dual-contouring method to a TDR file (see [Dual-Contouring Method on page 539](#)):

```
save type=dc [dc_min_angle=<n>] [dc_min_dihedral_angle=<n>] \
[dc_reference_volume_scaling=<n>] [dc_snap_to_box=<b>] \
[dc_version=<n>] [file=<c>] [include_grain_index=<b>] \
[keep_top_gas=<b>] [mean_spacing=<n>] [structure=<c>]
```

Save a PMC structure converted to a GC structure to a TDR file:

```
save [type=gc] [force_save=<b>] [gc_samples_per_cell=<n>] \
[structure=<c>] [tdr_geometry=<c>]
```

Extract the boundary of a PMC structure and save it to a TDR file:

```
save type=vbe [add_interfaces=<b>] [decimate=<b> [accuracy=<n>]] \
[file=<c>] [force_save=<b>] [grain_regions=<b>] \
[include_grain_index=<b>] [material_priority=<l>] \
[material_selection=<c>] [min_angle=<n>] [min_dihedral_angle=<n>] \
[ridge_angle=<n>] [shortest_edge=<n>] [structure=<c>] \
[tdr_geometry=<c>]
```

Save a PMC structure to a PMC file:

```
save type=pmc [file=<c>] [force_save=<b>] [initial_structure=<c>] \
[structure=<c>]
```

Chapter 6: Input Commands

save

Save the local pattern density, effective pattern density, and rate correction factor as a function of x and y in a TDR file:

```
save pattern_density_model=<c> [file=<c>] [point_max=<v>] \
[point_min=<v>]
```

Note:

If the plot domain is not specified explicitly by `point_min` and `point_max`, then it is automatically made large enough to contain all local pattern density regions, plus sufficient space to capture the decay of the effective pattern density function. Since saving large and complex pattern density maps can lead to excessive calculation times and output file size, you should always limit the output domain by setting `point_min` and `point_max` explicitly.

Save PMC damage in a tensor structure in a TDR file:

```
save type=transfer [file=<c>] [point_min=<n>] [point_max=<n>] \
[structure=<c>]
```

Save a PMC structure to a boundary structure in a TDR file by mapping mixed PMC cells to compound materials (the map or maps specified in `merge_replacements` are created in the `define_material_replacement` command):

```
save merge_replacements=<l> [file=<c>] [merge_tolerance=<n>] \
[structure=<c>]
```

Save a grid containing the volume fractions of the species in a PMC structure to a TDR file:

```
save type=volume_fractions [file=<c>] [force_save=<b>] \
[point_max=<v>] [point_min=<v>] [structure=<c>] [tdr_geometry=<c>]
```

When simulating charge-up, save a grid containing the charge density, electric potential, or electric field to a TDR file:

```
save type=charge_density \
[file=<c>] [force_save=<b>] [point_min=<v>] [point_max=<v>] \
[structure=<c>] [tdr_geometry=<c>]
```

```
save type=electric_field \
[file=<c>] [force_save=<b>] [point_min=<v>] [point_max=<v>] \
[structure=<c>] [tdr_geometry=<c>]
```

```
save type=electric_potential \
[file=<c>] [force_save=<b>] [point_min=<v>] [point_max=<v>] \
[structure=<c>] [tdr_geometry=<c>]
```

Save tabular NADs, tabular IADs, probability, reflection, and yield functions to a TDR file:

```
save nad=<c> [file=<c>] [force_save=<b>] [tdr_geometry=<c>]
```

```
save iad=<c> [file=<c>] [force_save=<b>] [tdr_geometry=<c>]
```

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save

```
save probability=<c> [file=<c>] [force_save=<b>] [<sampling_options>]  
save reflection=<c> [file=<c>] [force_save=<b>] [<sampling_options>]  
save yield=<c> [file=<c>] [force_save=<b>] [<sampling_options>]
```

Save the angular distributions or energy angular distributions (EADs) of species distributions to a TDR file:

```
save species_distribution=<c> [azimuth=<n>] \  
[file=<c>] [force_save=<b>] \  
[output_type=distribution] [<sampling_options>] [t=<n>]
```

Save the numeric parameters used to create the species distributions as a function of time to a TDR file:

```
save species_distribution=<c> output_type=parameters time=<n> \  
[file=<c>] [force_save=<b>]
```

Save species distributions in EAD file format (see [Appendix B on page 616](#)):

```
save species_distribution=<c> file_type=text species=<c> \  
[azimuth=<n>] [conversion_factor=<n>] \  
[distribution_format=<c>] \  
[file=<c>] [file_format=<c>] [force_save=<b>] \  
[<sampling_options>] [t=<n>] [version_number=<n>]
```

In the syntax, <sampling_options> denotes a set of optional sampling parameters for the energy- and angle-dependent functions:

```
<sampling_options>= \  
angle_max=<n> angle_min=<n> angle_samples=<n> \  
energy_max=<n> energy_min=<n> energy_samples=<n>
```

If you do not specify the energy bounds of the species distribution (energy_min, energy_max), then the bounds are computed automatically within a reasonable range for the given species distribution. You can adjust the precision of the EAD to be saved by increasing the number of angle samples and energy samples.

Note:

When saving an azimuth-dependent species distribution to a TDR file or an EAD text file, a 2D cross section of the distribution at constant azimuth (specified by parameter azimuth) is saved.

When saving time-dependent species distributions, you can use the parameter t to specify the time point at which to save the distribution.

When you start Sentaurus Topography 3D with the --processes command-line option with a value greater than 1 (see [Table 1 on page 18](#)), except when type=gc, the parameter structure must not denote a structure obtained from the etch command using method=pmc averaging_runs=1.

Chapter 6: Input Commands

save

Save the reaction rate coefficients, defined in your plasma model by the command `add_bulk_reaction` (see [add_bulk_reaction](#)), as a function of the electron temperature to a TDR file:

```
save plasma_model=<c> quantity=rate_coefficient \
[file=<c>] [force_save=<b>] \
[expression_pattern=<c> | reactions=<l>] \
[num_samples=<n>] [pattern_type=<c>] [regex_syntax=<c>] \
[temperature_max=<n>] [temperature_min=<n>]
```

Save the solution of a plasma simulation to a file:

```
save plasma_solution=<c> [file=<c>] [force_save=<b>]
```

Table 77 Parameters of save command

Parameter	Description
accuracy	Sets the maximum deformation during decimation of the boundary extracted with the VBE method relative to the mean PMC spacing. It can be specified only if <code>decimate=true</code> . Type: Number Default: <code>1e-3</code> Range: <code>[0, ∞[</code>
add_interfaces	If set to <code>true</code> , interface regions for the interface of bulk regions that touch each other are added. Type: Boolean Default: <code>false</code>
angle_max	Sets the upper end of the angle window to save. Type: Number Default: <code>90</code> Range: <code>[0, 90]</code> Unit: degree
angle_min	Sets the lower end of the angle window to save. Type: Number Default: <code>0</code> Range: <code>[0, 90]</code> Unit: degree

Chapter 6: Input Commands

save

Table 77 Parameters of save command (Continued)

Parameter	Description
angle_samples	Sets the number of angular samples to save. Type: Number Default: 90 if saving probability, reflection, or yield functions If saving species distributions, the default value is deduced automatically from the distribution Range: [2, 2147483647]
azimuth	Sets the azimuth angle ϕ at which the species distribution is saved ($\phi = 0$ corresponds to the x-axis of the simulation coordinate system). Type: Number Default: 0 Range: [-180, 180] Unit: degree
conversion_factor	Sets a global conversion factor that scales the EAD. Type: Number Default: 1 Range:]0, ∞ [
dc_min_angle	Sets the minimum angle of the surface mesh (see Dual-Contouring Method on page 539). Type: Number Default: Value of dc_min_angle parameter of let command Range: [0, 180] Unit: degree
dc_min_dihedral_angle	Sets the minimum dihedral angle of the surface mesh (see Dual-Contouring Method). Type: Number Default: Value of dc_min_dihedral_angle parameter of let command Range: [0, 180] Unit: degree
dc_reference_volume_scaling	When type=dc, this parameter allows you to adjust the surface location when converting a PMC structure to a boundary. Larger values expand the structure into the gas. Type: Number Default: none Range:]0, 2[Unit: unitless

Chapter 6: Input Commands

save

Table 77 Parameters of save command (Continued)

Parameter	Description
dc_snap_to_box	When <code>type=dc</code> and <code>dc_snap_to_box=true</code> , this parameter snaps the outer boundary points to the bounding box. This can help tools that read the boundary to create a bulk mesh. Type: Boolean Default: true
dc_version	Selects the version of the dual-contouring algorithm. Options are: <ul style="list-style-type: none">• 1: Selects the algorithm available in releases prior to S-2021.06.• 2: Selects the algorithm available starting from S-2021.06. Type: Number Default: 1
decimate	Specifies whether to decimate the boundary extracted with the VBE method. Type: Boolean Default: true
distribution_format	Sets the mathematical format of the distribution function. Options are: <ul style="list-style-type: none">• cos_convention• standard Type: Character Default: standard
energy_max	Sets the upper end of the energy window to save. Type: Number Default: 0 if saving probability, reflection, or yield functions If saving species distributions, the default value is deduced automatically from the distribution Range: [0, ∞[Unit: eV
energy_min	Sets the lower end of the energy window to save. Type: Number Default: 0 if saving probability, reflection, or yield functions If saving species distributions, the default value is deduced automatically from the distribution Range: [0, ∞[Unit: eV

Chapter 6: Input Commands

save

Table 77 Parameters of save command (Continued)

Parameter	Description
energy_samples	<p>Sets the number of energy samples to save.</p> <p>Type: Number</p> <p>Default: 100 if saving probability, reflection, or yield functions If saving species distributions, the default value is deduced automatically from the distribution</p> <p>Range: [2, 2147483647]</p>
expression_pattern	<p>Sets the search pattern that specifies which reaction equations are considered for plotting the rate coefficients. By default, the search pattern must be given in the glob syntax.</p> <p>To enter a regular expression instead, set <code>pattern_type=regex</code>. You can provide either a pattern or a list of reaction names (parameter <code>reactions</code>).</p> <p>You can specify this parameter only for <code>quantity=rate_coefficient</code>.</p> <p>Type: Character</p> <p>Default: none</p>
file	<p>Sets the path of the file where the data is saved.</p> <p>In the file name, <code><base_name></code> denotes the value of the <code>base_name</code> parameter of the <code>let</code> command.</p> <p>Type: Character</p> <p>Default: <code><base_name>.tdr</code> <code><base_name>.pmc</code> (if <code>type=pmc</code>) <code><base_name>.txt</code> (if <code>file_type=text</code>) <code><base_name>.plasma</code> (if <code>type=plasma</code>)</p>
file_format	<p>Sets the format of the EAD file.</p> <p>Type: Character</p> <p>Default: <code>ead_table</code></p>
file_type	<p>Sets the file type to use for saving the species distribution. Options are:</p> <ul style="list-style-type: none"> • <code>tdr</code> • <code>text</code> <p>Type: Character</p> <p>Default: <code>tdr</code></p>
force_save	<p>Specifies whether to produce output files even if Sentaurus Topography 3D was started with the <code>--no_save</code> command-line option.</p> <p>Type: Boolean</p> <p>Default: <code>false</code></p>

Chapter 6: Input Commands

save

Table 77 Parameters of save command (Continued)

Parameter	Description
gc_samples_per_cell	Sets the number of samples to take along the x- and y-directions per grid cell. Type: Number Default: 1 Range: [1, 2147483647]
grain_regions	Specifies whether the boundary structure produced by the VBE method should contain different regions for portions of the structure with the same material but with different material properties. Note: The VBE method can create boundary structures with no more than 240 regions. Type: Boolean Default: false
iad	Sets the name of the tabular IAD to be saved. Type: Character Default: none
include_disconnected_parts	Specifies whether to save the parts of the exposed surface lying above the topmost connected component of the exposed surface that divides the simulation domain into two half-spaces. Type: Boolean Default: true
include_grain_index	Specifies whether to save the material property (grain index in polycrystalline materials) as a field when saving PMC to brep structures using the VBE or DC method. If <code>include_grain_index=true</code> , then when saving from PMC to boundary format, the command writes the grain index as a field into the structure for the <code>filter_structure</code> command, or directly to the file for the <code>save</code> command. Best results are obtained using the <code>filter_structure</code> command with <code>decimate=false</code> to create a boundary with a fine mesh for viewing the field. Type: Boolean Default: false

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save

Table 77 Parameters of save command (Continued)

Parameter	Description
include_voids	Specifies whether to save the parts of the exposed surface lying below the topmost connected component of the exposed surface that divides the simulation domain into two half-spaces. Type: Boolean Default: true
initial_structure	Sets the name of the initial structure that is saved in the PMC file and can be used as the body for Boolean operations. Type: Character Default: none
keep_top_gas	Specifies whether to keep the top gas. This parameter applies only to the dual-contouring method (<code>type=dc</code>). See Dual-Contouring Method on page 539 . Type: Boolean Default: false
material_priority	Sets a material priority list for materials at interfaces when using the VBE method. Type: List Default: none
material_selection	Sets the algorithm used to select the materials of a PMC cell when using the VBE method (see Volume Boundary Extraction Method on page 539). Options are: <ul style="list-style-type: none">• maximum• mixed• proportional Type: Character Default: mixed
mean_spacing	When <code>type=dc</code> , this parameter sets the resolution of the dual-contouring boundary conversion method (see Dual-Contouring Method on page 539). Type: Number Default: Taken from most recent PMC step

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save

Table 77 Parameters of save command (Continued)

Parameter	Description
merge_replacements	<p>Specifies a list of material replacement maps defined in the command <code>define_material_replacement</code>. The list consists of the names of material replacement maps. PMC cells that contain the species matching the material replacement species and <code>volume_fractions</code> (with tolerance specified by <code>merge_tolerance</code>) are converted to the material specified by the material replacement map before the structure is saved.</p> <p>Note: This parameter can be used only with PMC structures.</p> <p>Type: List Default: none</p>
merge_tolerance	<p>Sets the allowed deviation from <code>volume_fractions</code> of the material replacement map, so as to perform the merge.</p> <p>Type: Number Default: 0.1</p>
min_angle	<p>Sets the smallest angle in the elements of the decimated surface of the extracted boundary structure.</p> <p>It can be specified only if <code>decimate=true</code>.</p> <p>Type: Number Default: 0 Range: [0, 180] Unit: degree</p>
min_dihedral_angle	<p>Sets the smallest dihedral angle between two elements, which share an edge, of the decimated surface of the extracted boundary structure.</p> <p>It can be specified only if <code>decimate=true</code>.</p> <p>Type: Number Default: 0 Range: [0, 180] Unit: degree</p>
nad	<p>Sets the name of the tabular NAD to be saved.</p> <p>Type: Character Default: none</p>

Chapter 6: Input Commands

save

Table 77 Parameters of save command (Continued)

Parameter	Description
num_samples	When saving the rate coefficient, this parameter sets the number of points used to resolve the rate coefficient curve. You can specify this parameter only for <code>quantity=rate_coefficient</code> . Type: Number Default: 1000 Range: [2, ∞)
output_type	Sets the type of output to produce when saving species distributions. Options are: <ul style="list-style-type: none">• distribution• parameters Type: Character Default: distribution
pattern_density_model	Sets the pattern density model defined in the command <code>define_pattern_density_model</code> (see define_pattern_density_model on page 295). Type: Character Default: none
pattern_type	When using <code>expression_pattern</code> to select the plasma reactions, this parameter sets the type of the pattern. Options are <code>glob</code> and <code>regex</code> . You can specify this parameter only for <code>quantity=rate_coefficient</code> . Type: Character Default: glob
plasma_model	Sets the name of the plasma model containing the reactions. Type: Character Default: none
plasma_solution	Sets the name of the plasma solution, which is saved to a file. The solution name is specified in the command <code>solve_reactor</code> . Type: Character Default: none

Chapter 6: Input Commands

save

Table 77 Parameters of save command (Continued)

Parameter	Description
point_max	<p>When saving the 2D pattern density, this parameter sets the upper-right corner coordinates {x y} of the domain.</p> <p>Otherwise, it sets the requested maximum corner of the bounding box of the grid containing the data. It can be set only when type=volume_fractions, charge_density, electric_field, or electric_potential.</p> <p>The actual maximum corner of the bounding box of the grid containing the data is obtained by snapping the given point_max value to a grid point of the PMC structure (specified with the parameter structure).</p> <p>Type: Vector Default: automatic Unit: μm</p>
point_min	<p>When saving the 2D pattern density, this parameter sets the lower-left corner coordinates {x y} of the domain.</p> <p>Otherwise, it sets the requested minimum corner of the bounding box of the grid containing the data. It can be set only when type=volume_fractions, charge_density, electric_field, or electric_potential.</p> <p>The actual minimum corner of the bounding box of the grid containing the data is obtained by snapping the given point_min value to a grid point of the PMC structure (specified with the parameter structure).</p> <p>Type: Vector Default: automatic Unit: μm</p>
probability	<p>Sets the name of the probability function to save.</p> <p>Type: Character Default: none</p>
quantity	<p>Sets the quantity to save from the specified plasma model.</p> <p>You can specify this parameter only when plasma_model is specified.</p> <p>The only value is rate_coefficient.</p> <p>Type: Character Default: none</p>

Chapter 6: Input Commands

save

Table 77 Parameters of save command (Continued)

Parameter	Description
reactions	<p>Specifies the names of the reactions whose rate coefficients should be plotted. If not specified, then all reactions are extracted.</p> <p>You can provide either a list of reaction names or a pattern for the reaction equation (parameter <code>expression_pattern</code>).</p> <p>You can specify this parameter only for <code>quantity=rate_coefficient</code>.</p> <p>Type: List Default: none</p>
reflection	<p>Sets the name of the reflection function to save.</p> <p>Type: Character Default: none</p>
regex_syntax	<p>When using <code>expression_pattern</code> with <code>pattern_type=regex</code> to select the plasma reactions, this parameter defines the syntax of the regular expression. Options are:</p> <ul style="list-style-type: none"> • extended • awk • basic • ecma_script • egrep • grep <p>You can specify this parameter only for <code>quantity=rate_coefficient</code>.</p> <p>Type: Character Default: extended</p>
ridge_angle	<p>Sets the angle used by the decimation algorithm to determine geometric features of the extracted boundary structure.</p> <p>It can be specified only if <code>decimate=true</code>.</p> <p>Type: Number Default: 179 Range: [0, 180] Unit: degree</p>
shortest_edge	<p>Sets the shortest edge of the decimated surface of the extracted boundary structure, relative to the mean PMC spacing.</p> <p>It can be specified only if <code>decimate=true</code>.</p> <p>Type: Number Default: Value set by the <code>accuracy</code> parameter Range: [0, ∞[</p>

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save

Table 77 Parameters of save command (Continued)

Parameter	Description
species	Sets the name of the species to save. Type: Character Default: none
species_distribution	Sets the name of the species distribution to save. Type: Character Default: none
structure	Sets the name of the structure to save. Type: Character Default: default_structure
t	Sets the time at which to save the species distributions. Type: Number Default: Number Range: [0, ∞[Unit: minute
tdr_geometry	Sets the name of the TDR geometry to save. Type: Character Default: none
temperature_max	Sets the upper limit of the plotting range when plotting the rate coefficient as a function of the electron temperature. You can specify this parameter only for quantity=rate_coefficient. Type: Number Default: 100 Range: [0, ∞[Unit: eV
temperature_min	Sets the lower limit of the plotting range when plotting the rate coefficient as a function of the electron temperature. You can specify this parameter only for quantity=rate_coefficient. Type: Number Default: 0 Range: [0, ∞[Unit: eV

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save

Table 77 Parameters of save command (Continued)

Parameter	Description
time	Sets the time until which to save the numeric parameters used to create the species distributions. Type: Number Default: none Range: [0, ∞[Unit: minute
type	Sets the type of data to save. Options are: <ul style="list-style-type: none">• charge_density• closed_surface• dc• electric_field• electric_potential• exposed_surface• final_structure• gc• pmc• transfer• vbe• volume_fractions Type: Character Default: gc if the parameter structure denotes a PMC structure; final_structure otherwise
version_number	Sets the version number of the EAD file. Type: Number Default: 0.0 Range: [0.0, ∞[
yield	Sets the name of the yield function to save. Type: Character Default: none

Note:

When `type=closed_surface`, or `type=exposed_surface`, or `type=final_structure`, the parameter structure cannot specify a PMC structure. To process such a structure, an explicit conversion of the structure is needed before calling the `save` command (see [Integration With Other Sentaurus Topography 3D Functionality on page 580](#)).

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save

When `type=gc`, `type=pmc`, `type=transfer`, `type=volume_fractions`, or `type=vbe`, the parameter structure must specify a PMC structure.

Saving Structures

As described in [Boundary Types on page 31](#), the following boundary types can be saved:

- Closed surface (`type=closed_surface`)
- Exposed surface (`type=exposed_surface`)
- Final structure (`type=final_structure`)

By default, the `save` command saves the final structure.

Note:

See [Integration With Other Sentaurus Topography 3D Functionality on page 580](#) for the limitations when saving a PMC structure.

The command `save` can be used more than once in the same command file. The first time that a file name (default name or user-defined name using the parameter `file`) is used, a new TDR file with that name is created or overwritten in the case where the file already exists from a previous simulation.

In subsequent uses of the `save` command that refer to the same file name, the results are appended to the previously saved structures in that file independently of the saved type or of the simulation step that preceded the `save` command. In other words, a file that is created within a simulation is never overwritten, and data is always appended to it.

You can save the resulting structure into a different file by creating a new file with the parameter `file`.

Examples

`save`

`save type=closed_surface`

The first `save` command saves the final structure into the default TDR file. The second `save` command adds the corresponding closed surface to the same file.

`save file="mosfet.tdr" tdr_geometry="pmos"`

This command saves the current structure to the TDR file `mosfet.tdr` and gives the created TDR geometry the name `pmos`. The name can be reused to load this specific geometry in the `define_structure` command, for example.

Chapter 6: Input Commands

save

Saving Ion Angular Distributions

The `save` command can save ion angular distributions (IADs) to TDR files.

Examples

Save the IAD named `iad_1` to the default TDR file:

```
save iad=iad_1
```

Save the IAD `iad_1` to the file `iad1.tdr`, and name the IAD in the file `ion_iad`:

```
save iad=iad_1 file=iad1.tdr tdr_geometry=ion_iad
```

Saving PMC Structures

A PMC structure is stored in a PMC file with the `save` command when `type=pmc`.

The advantage of using PMC files to create splits in a process flow, compared to TDR files containing boundaries, is that no conversion to a boundary and back to the PMC representation is required. Therefore, loading and saving is more efficient and does not introduce artifacts.

To perform Boolean operations and to create a boundary from a PMC structure that has been loaded from a PMC file, the initial structure from which the PMC structure has been created is required. The parameter `initial_structure` is used to specify the initial structure that is stored in the PMC file.

Note:

A PMC file is not a TDR file and cannot be visualized with Sentaurus Visual. It can only be loaded in to Sentaurus Topography 3D.

Examples

```
etch time=0.5 spacing=0.05 method=pmc machine=m_100  
save file=pmc_only.pmc type=pmc
```

The first command etches a structure using the PMC method. The second command saves the PMC structure to a PMC file without saving the initial structure to the PMC file.

Therefore, this PMC file can be used only as a starting point for other PMC simulations. It is not possible to perform Boolean operations or to convert the PMC structure to a boundary.

```
define_structure pmc_file=pmc_only.pmc  
etch time=0.5 spacing=0.05 method=pmc machine=m_100
```

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save

Here, the previously saved PMC structure is loaded from a PMC file and used for a PMC simulation.

```
define_structure material=Silicon point_min={0 0 0} point_max={1 1 1}
filter_structure type=copy name=sc
etch time=0.5 spacing=0.05 method=pmc machine=m_100
save file=pmc_and_initial.pmc type=pmc initial_structure=sc
```

In this example, an initial structure is created and copied to a structure named `sc`. After etching the initial structure, it is saved to a PMC file together with the boundary of the copy of the initial structure.

```
define_structure pmc_file=pmc_and_initial.pmc
etch time=0.5 spacing=0.05 method=pmc machine=m_100
filter_structure type=boolean body=sc
save file=f.tdr
```

In the first command, the PMC structure and the initial structure are loaded from a PMC file. After etching the PMC structure, Boolean operations are performed with the initial structure named `sc` loaded from the PMC file. Finally, the structure is saved as a boundary to a TDR file.

If the name of the initial structure stored in the PMC file is unknown, a new name can be specified with the parameter `initial_structure_name` as demonstrated in the following example:

```
define_structure pmc_file=pmc_and_initial.pmc \
    initial_structure_name=xyz
etch time=0.5 spacing=0.05 method=pmc machine=m_100
filter_structure type=boolean body=xyz
save file=f.tdr
```

Saving Boundaries for PMC Structures

To save a boundary structure for a PMC structure that has been created from a boundary structure using a PMC etch or deposition model, you can create a new boundary structure using `filter_structure type=boolean` and the initial boundary structure. The advantage of this method is that artifacts are limited to the parts of the structure that were modified by process steps. However, this method is computationally expensive.

There are alternative methods for saving a boundary structure that extract a boundary structure from a PMC structure without using the initial boundary structure:

- Dual-contouring method [17][18][19]
- Volume boundary extraction (VBE) method

The advantage of these methods is that they are computationally more efficient than the previously described method. However, when using either alternative method, conversion

Chapter 6: Input Commands

save

artifacts might be created throughout the entire structure, not only in the parts modified by process steps.

Dual-Contouring Method

Converting a PMC structure to a boundary structure using the dual-contouring method generally works well, but the conversion time and shape of the final boundaries can be fine-tuned with the parameters of the `save` command. To use the default parameter values, you only need to specify:

```
save type=dc
```

The main parameter that controls boundary fidelity is `mean_spacing`. The default of this parameter is the spacing used for the most recent PMC step. Specifying a smaller mean spacing leads to a more accurate boundary conversion; whereas, a larger mean spacing reduces runtime.

Note:

Do not specify `mean_spacing` less than approximately $\frac{1}{4}$ of the spacing used in the most recent PMC step because smaller spacing is not likely to improve the boundary fidelity further, but it is more likely to result in large runtimes.

The parameters `dc_min_angle` and `dc_min_dihedral_angle` can improve volume meshes in TCAD tools reading the boundary file. In most cases, the dual-contouring algorithm satisfies those criteria without compromising the boundary fidelity or introducing artifacts. However, a very high minimum dihedral angle threshold ($> 30^\circ$) might not be satisfied and can result in distortion or a slightly higher vertex count.

An improved version of the dual-contouring algorithm is available, which generates boundaries of a higher fidelity on interfaces and triple lines. It is also more effective at fitting the structure to the bounding box while satisfying the fidelity and quality shape criteria. These improvements might require additional computation time, which is usually less than 30%. The default version of the dual-contouring algorithm is the same as in releases prior to S-2021.06. To specify the improved version of the dual-contouring algorithm, specify `dc_version=2` either in the `filter_structure` command or in the `save` command.

Volume Boundary Extraction Method

The VBE method can also be used to save boundary structures for structures that were initially created as PMC structures.

Converting a PMC structure to a boundary structure using the VBE method might introduce artifacts at material interfaces due to the different discretization methods. The parameters `material_priority` and `material_selection` provide some control over the selection of materials at the interface of different materials.

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save

When using the material selection algorithm:

- If `material_selection=maximum`, the entire volume of a PMC cell is considered to be of the material that has the maximum partial volume.
- If `material_selection=proportional`, each material in a PMC cell is initially represented proportionally to its partial volume. Because the final result also depends on the materials in neighboring cells, materials for which the partial volume is less than 50% might be replaced by a different material.
- If `material_selection=mixed`, the effect is similar to `proportional`, but if the partial volume of the material with the highest partial volume in a cell is less than 50%, the partial volume is increased to 50% to ensure that this material is not replaced by a different material in the final result.

When two materials have the same partial volume in a cell, preference is given to the material with the higher priority. The parameter `material_priority` can specify materials according to their priority. The material listed first has the highest priority. Materials that are not in the list have lower priority than any of the listed materials.

Saving Species Distributions

The `save` command can save species distributions (EADs and angular distributions) to TDR files or EAD files.

The following command saves the EAD of a species distribution named `sd` in the energy range from 100 eV to 200 eV to the default TDR file:

```
save species_distribution=sd energy_min=100 energy_max=200
```

To save the angular distribution of a species distribution named `sd` at a certain energy level (for example, 100 eV) to the default TDR file, you must set `energy_min` and `energy_max` to the same value:

```
save species_distribution=sd energy_min=100 energy_max=100
```

You can change the default resolution of the saved EAD by specifying the number of energy and angle samples:

```
save species_distribution=sd angle_samples=180 energy_min=100 \
      energy_max=200 energy_samples=200
```

Accordingly, to change the default resolution of the angular distribution at energy 100 eV, specify:

```
save species_distribution=sd angle_samples=180 energy_min=100 \
      energy_max=100
```

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save

The following command saves the species distribution to an EAD file:

```
save species_distribution=sd species=Ar file_type=text
```

You can change the default EAD file format, the format of the distribution, the conversion factor, the version number, the energy bounds, and the number of energy samples and angle samples:

```
save species_distribution=sd species=Ar file_type=text \
angle_samples=180 conversion_factor=10 version_number=1.1 \
distribution_format=cos_convention energy_min=10 \
energy_max=200 energy_samples=500 file_format=ead_table \
```

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set_field

set_field

This command sets the value of a field on a given PMC structure, as specified by an analytic expression.

Note:

The command works only for PMC structures.

Syntax

```
set_field expression=<c> field=<c> [structure=<c>]
```

Table 78 Parameters of set_field command

Parameter	Description
expression	Specifies a position-dependent expression for the value to be set for the field specified by the parameter field . For details about position-dependent expressions, see Syntax for Expressions on page 139 . Type: Character Default: None Range: [0, 1] when field=activation , or [0, ∞[when field=recoil or field=vacancy
field	Specifies the name of the field for which to set its value. Options are: <ul style="list-style-type: none">• activation• recoil• vacancy Type: Character Default: none
structure	Sets the name of a PMC structure for which to set the field. Type: Character Default: default_structure

Examples

Set the values of the **activation** field of the PMC structure named **default_structure** as specified by an analytic function of the position:

```
set_field field=activation \
    expression="min(1, max(0, 1 / (1 + x * x + y * y + z * z)))"
```

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set_material_properties

set_material_properties

This command sets the crystal material properties for a material or a region in a structure.

Note:

For this command:

- The material of structures defined using `define_structure material=<c> point_min=<v> point_max=<v> [structure=<c>] ...` is amorphous.
- The materials added using the commands `deposit shape=<c> ...`, `fill`, and `pattern` are amorphous.

Syntax

For 3D boundary and GC structures:

```
set_material_properties material=<c> type=<c> <material_properties> \
[structure=<c>]

set_material_properties region=<c> type=<c> <material_properties> \
[structure=<c>]
```

For PMC structures:

```
set_material_properties material=<c> type=<c> <material_properties> \
[structure=<c>]
```

Table 79 Parameters of set_material_properties command

Parameter	Description
anisotropy_xz, anisotropy_yz	Specify the ratio of the average grain size in x, with respect to z. The average grain size in x is <code>anistropy_xz * average_grain_size</code> and, similarly, for y <code>anistropy_yz * average_grain_size</code> . Type: Number Default: 1 Range:]0, ∞[
average_grain_size	Sets the average size of the polycrystalline material grains. Type: Number Default: none Range:]0, ∞[Unit: µm

Chapter 6: Input Commands

set_material_properties

Table 79 Parameters of set_material_properties command (Continued)

Parameter	Description
crystal_type	Sets the crystal type of crystalline or polycrystalline materials. The only supported option is diamond. Type: Character Default: none
flat_orientation	Sets the Miller index of the direction perpendicular to the wafer flat (y-axis of the wafer coordinate system) for the material or region. Note: The direction specified by this parameter must be orthogonal to the direction specified by the parameter vertical_orientation. Type: Vector Default: none
lattice_constant	Sets the lattice constant of the crystal for crystalline or polycrystalline materials. Type: Number Default: 0.5431020511e-3 Range:]0, ∞[Unit: μm
material	Sets the name of the material for which the properties are set. Type: Character Default: none
<material_properties>	Denotes a set of parameters dependent on the value of parameter type, as specified in Table 80 . Type: Character Default: none
preferred_vertical_orientation	Sets the Miller index of the grain-preferred direction perpendicular to the wafer surface (z-axis of the wafer coordinate system) for the material or region. If omitted, then grain orientations are distributed uniformly. Type: Vector Default: none
region	Sets the name of the region for which the properties are set. Type: Character Default: none

Chapter 6: Input Commands

set_material_properties

Table 79 Parameters of set_material_properties command (Continued)

Parameter	Description
structure	Sets the name of the structure for which the properties are set. Type: Character Default: default_structure
type	Sets the type of the material. Options are: <ul style="list-style-type: none">• amorphous• crystalline• polycrystalline Type: Character Default: none
vertical_orientation	Sets the Miller index of the direction perpendicular to the wafer surface (z-axis of the wafer coordinate system) for the material or region. Note: The direction specified by this parameter must be orthogonal to the direction specified by flat_orientation. Type: Vector Default: none
vertical_orientation_spread	Sets the angle of allowed deviation from the preferred orientation for polycrystalline materials. Type: Number Default: 10 Range: [1, 90] Unit: degree

Table 80 Material properties: type dependent

type	<material_properties>
amorphous	No parameters
crystalline	crystal_type=<c> flat_orientation=<v> vertical_orientation=<v> [lattice_constant=<n>]
polycrystalline	crystal_type=<c> average_grain_size=<n> [anisotropy_xz=<n>] [anisotropy_yz=<n>] [lattice_constant=<n>] [preferred_vertical_orientation=<v>] [vertical_orientation_spread=<n>]

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set_material_properties

Examples

Make material Oxide of structure default_structure amorphous:

```
set_material_properties material=Oxide type=amorphous
```

Make material Silicon of structure default_structure crystalline with a diamond crystal structure and crystal orientation such that:

- When cutting the material with a plane parallel perpendicular to the y-axis of the wafer coordinate system, a (1 1 0) plane is exposed
- When cutting the material with a plane parallel perpendicular to the z-axis of the wafer coordinate system, a (0 0 1) plane is exposed

```
set_material_properties material=Silicon type=crystalline \
    crystal_type=diamond flat_orientation={1 1 0} \
    vertical_orientation={0 0 1}
```

Make material Silicon of structure default_structure polycrystalline with grains of an average size of 0.1 mm and (0 0 1) as the preferred vertical orientation with an angular spread of 15°:

```
set_material_properties material=Silicon type=polycrystalline \
    crystal_type=diamond \
    preferred_vertical_orientation={0 0 1} \
    vertical_orientation_spread=15
```

Chapter 6: Input Commands

set_orientation

set_orientation

This command is used to set or change the crystal orientation of a region.

Syntax

```
set_orientation flat_orientation=<v> region=<c> \
    vertical_orientation=<v> [structure=<c>]
```

Table 81 Parameters of set_orientation command

Parameter	Description
flat_orientation	Sets the Miller index of the direction perpendicular to the wafer flat (y-axis of the wafer coordinate system) for this region. Type: Vector Default: none
region	Sets the name of the region for which the crystal orientation is set. Type: Character Default: none
structure	Sets the name of the structure whose crystal orientation must be set. Type: Character Default: default_structure
vertical_orientation	Sets the Miller index of the direction perpendicular to the wafer surface (z-axis of the wafer coordinate system) for this region. Type: Vector Default: none

Chapter 6: Input Commands

solve_reactor

solve_reactor

This command executes the plasma model solvers, that is, it solves the plasma bulk and plasma sheath models defined in the plasma model.

Syntax

```
solve_reactor name=<c> reactor=<c> \
    [bulk_solver=<c>] [extractions=<l>] [sheath_solver=<c>]
```

Table 82 Parameters of solve_reactor command

Parameter	Description
bulk_solver	Sets the name of the plasma bulk solver to be used for solving the plasma model. It must have been already defined in the define_bulk_solver command (see define_bulk_solver on page 210). Type: Character Default: default_global_bulk_solver
extractions	Specifies a list of the names of extractions to be used when solving the plasma model. Each name in the list must have been already defined in the define_extraction command (see define_extraction on page 252). Type: List Default: none
name	Sets the name of the plasma solution. The name is used for later reference, for example, in the define_reactor or define_species_distribution command (see define_reactor on page 301 and define_species_distribution on page 337). Type: Character Default: none
reactor	Sets the name of the plasma reactor (as defined in the define_reactor command), which contains the equipment parameters and the plasma model to be solved (see define_reactor on page 301). Type: Character Default: none
sheath_solver	Sets the name of the plasma sheath solver to be used for solving the plasma model, as defined in the command define_sheath_solver (see define_sheath_solver on page 330). Type: Character Default: Depends on the sheath model type defined in the plasma model: default_analytic_sheath_solver or default_circuit_sheath_solver

Chapter 6: Input Commands

solve_reactor

Examples

```
solve_reactor name=sol1 reactor=R  
  
solve_reactor name=sol1 reactor=R \  
    bulk_solver=default_global_bulk_solver  
  
solve_reactor name=sol1 reactor=R bulk_solver=s1 sheath_solver=s2
```

Note:

The solution computed by the `solve_reactor` command is stored internally and can be referenced by the `name` parameter in other commands, such as `save` and `define_species_distribution`. Some scalar quantities of the solution are also returned as a Tcl list, for example, the bulk densities, the electron temperature, the species fluxes, and so on. For example:

```
set res [solve_reactor name=sol1 reactor=R]  
puts $res  
>>> {{Ar+_density 2.85574e+17} {Ar+_energy_max 45.4943}  
{Ar+_energy_min 13.6602} {Ar+_flux 0.000779226}  
{e-_temperature 3.00445} ...}
```

Chapter 6: Input Commands

transform_structure

transform_structure

This command performs an axis-mapping transformation on structures, that is, it remaps one axis onto another, changing the coordinate system of the structure.

If you set only one target axis, then the other axis is set automatically to the other axis with the same sign. For example, if you set only `target_y_axis= -x`, then `target_x_axis= -y` is set automatically.

Note:

The `axis_mapping` transformation works only for 2D brep structures.

Syntax

```
transform_structure type=<c> [name=<c>] [structure=<c>] \
[target_x_axis=<c>] [target_y_axis=<c>]
```

Table 83 Parameters of `transform_structure` command

Parameter	Description
<code>name</code>	Sets the name of the transformed structure. If not set, then the input structure is replaced with the transformed structure. Type: Character Default: none
<code>structure</code>	Sets the name of the input structure. Type: Character Default: <code>default_structure</code>
<code>target_x_axis</code>	Sets the target x-axis. Options are: <ul style="list-style-type: none">• <code>x</code>• <code>-x</code>• <code>y</code>• <code>-y</code> The parameters <code>target_x_axis</code> and <code>target_y_axis</code> cannot reference the same axis. Type: Character Default: none

Chapter 6: Input Commands

transform_structure

Table 83 *Parameters of transform_structure command (Continued)*

Parameter	Description
target_y_axis	<p>Sets the target y-axis. Options are:</p> <ul style="list-style-type: none">• x• -x• y• -y <p>The parameters <code>target_x_axis</code> and <code>target_y_axis</code> cannot reference the same axis.</p> <p>Type: Character Default: none</p>
type	<p>Sets the type of transformation to be performed. The only option is <code>axis_mapping</code>.</p> <p>Type: Character Default: none</p>

Examples

```
transform_structure type=axis_mapping target_x_axis= -y
```

Chapter 6: Input Commands

truncate

truncate

This command truncates a structure, removing everything that lies outside of a cuboid bounding box.

Note:

When you start Sentaurus Topography 3D with the `--processes` command-line option with a value greater than 1 (see [Table 1 on page 18](#)), the parameter structure must not denote a structure obtained from the `etch` command using `method=pmc averaging_runs=1`.

Syntax

Truncate a boundary structure:

```
truncate point_min=<v> point_max=<v> \
[accuracy=<n>] [comment=<c>] [decimate=<b>] [min_angle=<n>] \
[min_dihedral_angle=<n>] [ridge_angle=<n>] [shortest_edge=<n>] \
[structure=<c>]
```

Truncate a PMC structure:

```
truncate point_min=<v> point_max=<v> [comment=<c>] [structure=<c>]
```

Table 84 Parameters of `truncate` command

Parameter	Description
accuracy	<p>Sets the maximum deviation between the decimated surface of the boundary structure produced by Boolean operations and its original surface.</p> <p>When set to -1, the used value is half of the structure-dependent spacing <code>epsilon</code>¹.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none">• The <code>structure</code> parameter denotes a boundary structure.• You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_accuracy=<n></code> Range: $\{-1\} \cup [0, \infty[$ Unit: μm</p>

Chapter 6: Input Commands

truncate

Table 84 Parameters of truncate command (Continued)

Parameter	Description
comment	Sets a comment for this process step that will be displayed or written to the log file. Type: Character Default: empty string
decimate	Specifies whether to decimate the boundary structure produced by Boolean operations. It can be specified only if <code>structure</code> denotes a boundary structure. Type: Boolean Default: Value set by <code>let decimate=</code>
min_angle	Sets the smallest angle in the elements of the decimated surface of the boundary structure produced by Boolean operations. This parameter can be specified only if all of the following conditions are met: <ul style="list-style-type: none"> The <code>structure</code> parameter denotes a boundary structure. You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. Type: Number Default: Value set by <code>let decimate_min_angle=<n></code> Range: [0, 180] Unit: degree
min_dihedral_angle	Sets the smallest dihedral angle between two elements of the decimated surface of the boundary structure produced by Boolean operations that share an edge. This parameter can be specified only if all of the following conditions are met: <ul style="list-style-type: none"> The <code>structure</code> parameter denotes a boundary structure. You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. Type: Number Default: Value set by <code>let decimate_min_dihedral_angle=<n></code> Range: [0, 180] Unit: degree

Chapter 6: Input Commands

truncate

Table 84 Parameters of truncate command (Continued)

Parameter	Description
point_max	<p>Sets the maximum corner point of the bounding cube. When truncating a PMC structure, the actual maximum corner of the truncated PMC structure is obtained by snapping the <code>point_max</code> value to a grid point of the input PMC structure.</p> <p>Type: Vector Default: none Unit: μm</p>
point_min	<p>Sets the minimum corner point of the bounding cube. When truncating a PMC structure, the actual minimum corner of the truncated PMC structure is obtained by snapping the <code>point_min</code> value to a grid point of the input PMC structure.</p> <p>Type: Vector Default: none Unit: μm</p>
ridge_angle	<p>Sets the angle used by the decimation algorithm to determine geometric features of the boundary structure produced by Boolean operations. This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none">• The <code>structure</code> parameter denotes a boundary structure.• You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_ridge_angle=<n></code> Range: [0, 180] Unit: degree</p>

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truncate

Table 84 Parameters of truncate command (Continued)

Parameter	Description
shortest_edge	<p>Sets the shortest edge of the decimated surface of the boundary structure produced by Boolean operations.</p> <p>When set to -1, the used value is half of the structure-dependent spacing epsilon¹.</p> <p>This parameter can be specified only if all of the following conditions are met:</p> <ul style="list-style-type: none"> The <code>structure</code> parameter denotes a boundary structure. You specify <code>decimate=true</code> or, if you do not specify <code>decimate</code>, you did not specify <code>let decimate=false</code>. <p>Type: Number Default: Value set by <code>let decimate_shortest_edge=<n></code> Range: $\{-1\} \cup [0, \infty[$ Unit: μm</p>
structure	<p>Sets the name of the structure that must be truncated.</p> <p>Note: This parameter cannot specify a PMC structure. To process such a structure, an explicit conversion of the structure is needed before calling the <code>truncate</code> command (see Integration With Other Sentaurus Topography 3D Functionality on page 580).</p> <p>Type: Character Default: <code>default_structure</code></p>

1. *The structure-dependent spacing epsilon is logged out when defining a structure using the `define_structure` command.*

Examples

Remove all parts of a structure that are outside a bounding box with the specified corners $\{0\ 0\ 0\} \ \{1\ 1\ 1\}$:

```
truncate point_min={0 0 0} point_max={1 1 1} comment="truncation"
```

The comment for this process step is displayed in the log file.

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7

Integration With Sentaurus Process and Sentaurus Interconnect

This chapter describes the integration of Sentaurus Topography 3D functionality into Sentaurus Process and Sentaurus Interconnect.

The Sentaurus Process and Sentaurus Interconnect executables support a subset of Sentaurus Topography 3D commands for advanced etching and deposition modeling. This integration allows the users of Sentaurus Process and Sentaurus Interconnect to easily incorporate one or more etching and deposition process steps into their simulation flow without having to create a separate command file and simulation node for Sentaurus Topography 3D.

Not all commands of Sentaurus Topography 3D are supported in Sentaurus Process and Sentaurus Interconnect, however.

Note:

For brevity, in this chapter, whenever *Sentaurus Process* is mentioned, it implicitly means *Sentaurus Process and Sentaurus Interconnect*.

Supported Commands and Syntax

Sentaurus Topography 3D functionality is accessible using the `topo` command in Sentaurus Process. The `topo` command acts as a prefix and branches into a subset of Sentaurus Topography 3D commands. In general, the `topo` command is followed by the Sentaurus Topography 3D subcommand.

For example, the following command calls the Sentaurus Topography 3D `etch` command from Sentaurus Process (the parameters are the same as for the original `etch` command):

```
topo etch spacing= {0.1} time=1.0
```

The syntax of the Sentaurus Topography 3D subcommands is the same as in Sentaurus Topography 3D (see [Chapter 6 on page 137](#)).

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Supported Commands and Syntax

Table 85 Sentaurus Topography 3D commands supported from within Sentaurus Process

Sentaurus Topography 3D command	Sentaurus Process command
add_bulk_reaction	topo add_bulk_reaction
add_float_parameter	topo add_float_parameter
add_flux_properties	topo add_flux_properties
add_formula	topo add_formula
add_int_parameter	topo add_int_parameter
add_ion_flux	topo add_ion_flux
add_material	topo add_material
add_neutral_flux	topo add_neutral_flux
add_reaction	topo add_reaction
add_reaction_properties	topo add_reaction_properties
add_source_species	topo add_source_species
add_species	topo add_species
define_bulk_solver	topo define_bulk_solver
define_deposit_machine	topo define_deposit_machine
define_etch_machine	topo define_etch_machine
define_iad	topo define_iad
define_model	topo define_model
define_plasma_model	topo define_plasma_model
define_probability	topo define_probability
define_reactor	topo define_reactor
define_reflection	topo define_reflection
define_sheath_solver	topo define_sheath_solver

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Additional Supported Parameters

Table 85 *Sentaurus Topography 3D commands supported from within Sentaurus Process*

Sentaurus Topography 3D command	Sentaurus Process command
define_species_distribution	topo define_species_distribution
define_species_properties	topo define_species_properties
define_yield	topo define_yield
deposit	topo deposit
etch	topo etch
finalize_model	topo finalize_model
solve_reactor	topo solve_reactor

Additional Supported Parameters

The `topo` command and Sentaurus Topography 3D subcommands in Sentaurus Process support some parameters that are exclusive to Sentaurus Process.

The info Parameter

This parameter sets the verbosity of the output of a command. See the *Sentaurus™ Process User Guide* for details.

Example

Call the `etch` command from Sentaurus Process with a verbosity level of 3:

```
topo etch spacing= {0.1} time=1.0 info=3
```

The parameters Parameter

This parameter prints a list of all the supported subcommands and their syntax.

Example

Print the syntax of all the supported Sentaurus Topography 3D subcommands:

```
topo parameters
```

The repair Parameter

The `topo etch` and `topo deposit` commands support the `repair` parameter, which switches on boundary repair for etching and deposition steps. By default, boundary repair is switched on. See the *Sentaurus™ Process User Guide* for details.

Example

Call the `topo deposit` command with boundary repair deactivated:

```
topo deposit spacing= {0.1} time=1.0 !repair
```

Different Default Behavior

To ensure consistent behavior of the Sentaurus Topography 3D commands when they are called from Sentaurus Process, some commands have different default behavior. These commands behave slightly differently when called from Sentaurus Topography 3D or Sentaurus Process.

Boundary Repair

The boundary repair behavior differs as follows:

- Sentaurus Topography 3D default behavior: Boundary repair is deactivated because it can use excessive CPU time and memory. You can activate boundary repair using the command:

```
let snmesh_repair=true
```

- Sentaurus Process default behavior: Boundary repair for `topo etch` and `topo deposit` is activated (see [The repair Parameter](#)).

Region Merging

Both when calling the `topo` command from Sentaurus Process and when using Sentaurus Topography 3D directly, regions with the same materials are not merged by default.

This behavior is different from deposition using the MGOALS module in Sentaurus Process, where regions merge by default.

To activate region merging in the `topo` command, use the `merge` parameter in the `deposit` and `etch` commands (see [deposit on page 375](#) and [etch on page 399](#)).

Parallelization

Parallelization differs as follows:

- In standalone Sentaurus Topography 3D, the `let num_threads` and `let parallel` commands as well as the command-line options `--max_threads` and `--threads` are used to activate shared-memory parallelization and to control the number of threads (see [From the Command Line on page 17](#) and [let on page 501](#)).
- In Sentaurus Process, the `math` command controls shared-memory parallelization. The `topo` command uses the number of threads defined with the `math` command. See the *Sentaurus™ Process User Guide* for details about parallelization.

Limitations and Known Issues

There are limitations when using Sentaurus Topography 3D from Sentaurus Process.

Boundary Conditions

In Sentaurus Topography 3D, boundary conditions are set using the command `define_boundary_conditions`, which is not a supported subcommand of the `topo` command. Therefore, only the default boundary conditions can be used from within Sentaurus Process.

Meshing Thin Layers

In standalone mode, Sentaurus Topography 3D creates boundary files as a result of process steps. Sentaurus Process, however, needs 3D meshes for most of its functionality. Boundaries are transferred from the `topo` command to Sentaurus Process automatically, and they are meshed when needed using Sentaurus Process commands such as `implant`.

Meshing of very thin material layers can be difficult. Meshing might either take a very long time or terminate if Sentaurus Mesh cannot mesh the structure.

Sentaurus Topography 3D often generates thin layers, especially in models where redeposition effects are modeled (for example, when using the `etchdepo` model).

The stop_function Parameter

The parameter `stop_function` and related parameters (`stop_function_interval`, `stop_function_times`, and `stop_function_times_unit`) of the `etch` command are not supported when calling the `etch` command from Sentaurus Process (see [etch on page 399](#)).

8

Rate Formula Module

This chapter describes the rate formula module.

Introduction to the Rate Formula Module

The rate formula module (RFM) allows you to define deposition and etching models in Sentaurus Topography 3D. In contrast to the physical model interface (PMI), which requires C++ programming, the RFM uses only built-in commands. Therefore, the RFM simplifies the development of new models and provides greater flexibility in modeling.

You can specify the deposition and etching rate by writing a mathematical formula. This formula can involve fluxes, geometric quantities of the surface, user-defined parameters, and mathematical functions. It is used in each time step as described in [Sentaurus Topography 3D Computational Model on page 23](#).

There are three distinct stages when using an RFM model, as illustrated in [Figure 35](#):

- *Model definition*

First, you define the model by specifying the fluxes used by the RFM model, the global and material-specific parameters, and the formulas for the etching or deposition rate. See [Model Definition on page 565](#).

- *Machine configuration*

Second, you define a machine that uses the newly defined model. See [Machine Configuration on page 569](#).

- *Machine use*

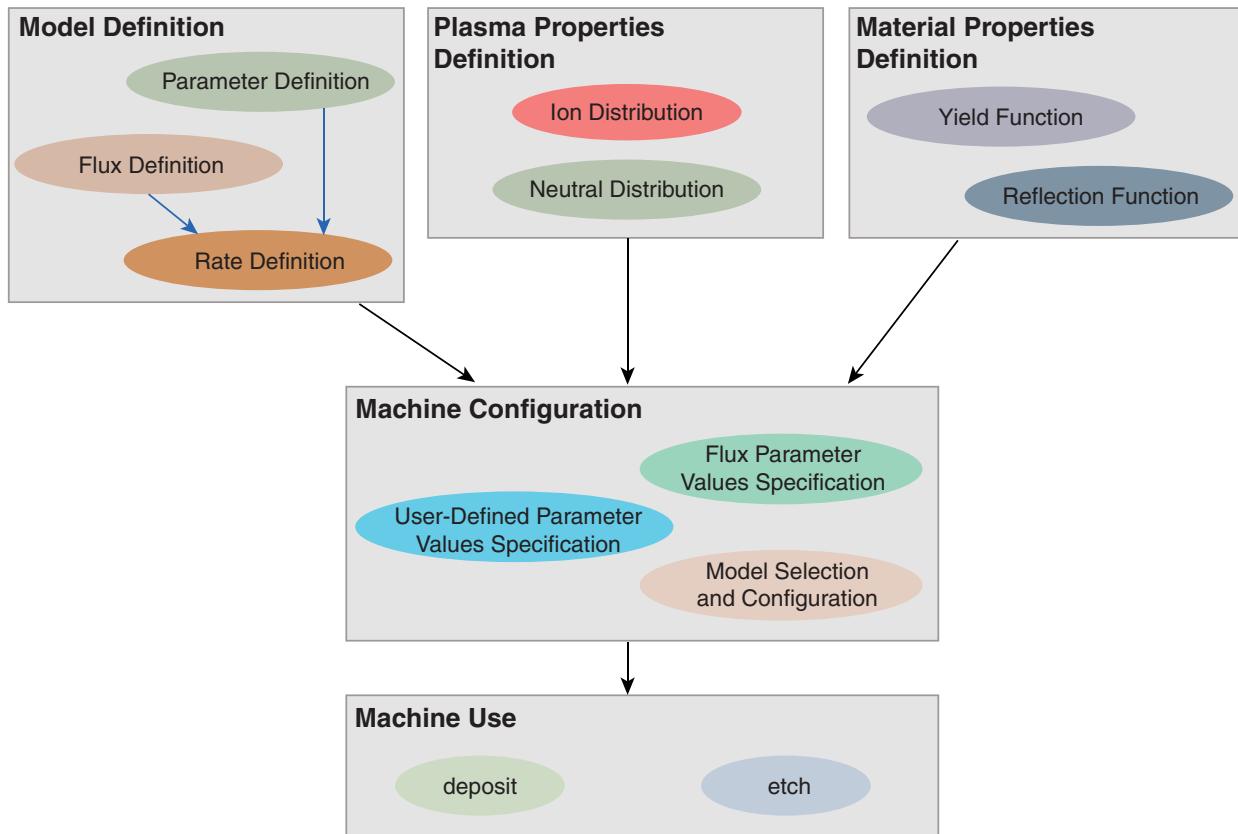
Finally, you use the machine with an `etch` or a `deposit` command. This is performed in exactly the same way as with machines that use built-in or PMI models (see [deposit on page 375](#) and [etch on page 399](#)).

Refer to the examples of how to create models using the RFM in the Sentaurus Topography 3D module of the TCAD Sentaurus Tutorial (see [TCAD Sentaurus Tutorial: Simulation Projects on page 21](#)).

Chapter 8: Rate Formula Module

Model Definition

Figure 35 RFM modeling flow



Model Definition

You define the model by specifying the fluxes used by the RFM model, the global and material-specific parameters, and the formulas for the etching or deposition rate. This stage is analogous to the creation of a PMI model where the new model is defined in the form of C++ code. Since there is only a small number of commands for defining a new model, it is much easier to learn how to create an RFM model than a PMI model.

You can add an arbitrary number of ion and neutral fluxes to an RFM model. The ion fluxes can be configured individually to take the physical effects of reflection, sputtering, and reemission into account. [Modeling Fluxes and Related Physical Effects on page 44](#) describes these physical effects and how they are calculated.

In general, deposition and etching models have parameters that are used to adjust the deposition and etching rates to specific process conditions. An arbitrary number of material-specific and global parameters can be added to an RFM model. During the

Chapter 8: Rate Formula Module

Model Definition

machine configuration, the values of these parameters can be set in the command file in the same way as for built-in and PMI models.

At each time step, Sentaurus Topography 3D calculates the rate of each surface element. For an RFM model, the rate is calculated from a user-defined mathematical expression. This expression can contain the values of the previously defined fluxes, the values of user-defined parameters, mathematical functions, and arithmetic operators.

Defining a Model

The definition of a model consists of five steps, two of which are optional:

1. You start with the `define_model` command, which provides the name and the type of the model (`deposit`, `etch`, or `etchdepo`), as well as a short description of the model.
2. (Optional) For models that depend on neutral and ion fluxes, you add these with the `add_neutral_flux` and `add_ion_flux` commands, respectively. See [Defining Fluxes](#).
3. (Optional) You add the floating-point and integer parameters used in the rate formula with the `add_float_parameter` and `add_int_parameter` commands, respectively. See [Specifying User-Defined Parameters on page 567](#).
4. You must specify a rate formula as a mathematical expression with the `add_formula` command. See [Defining a Rate Formula on page 568](#).
5. The model definition is marked as complete by specifying the `finalize_model` command.

Defining Fluxes

This step introduces the ion and neutral fluxes involved in the model and states which physical effects are taken into account for ion fluxes. For neutral fluxes, reemission is always activated, as discussed in [Modeling Fluxes and Related Physical Effects on page 44](#).

Neutral and ion fluxes are introduced by the `add_neutral_flux` and `add_ion_flux` commands, respectively, and the definition of each flux requires a unique identifier for the flux using the parameter `name` as well as the model to which the flux refers.

Accordingly, a neutral flux called `N` to be used in the model `my_model` is introduced with the statement:

```
add_neutral_flux model=my_model name=N
```

Typically, you set the value of the sticking coefficient of a neutral flux using the `add_flux_properties` command in the machine configuration. The value also can be specified with the `sticking` parameter in the `add_neutral_flux` command.

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Model Definition

It is important to note that, if the sticking coefficient of a neutral flux is set in the `add_neutral_flux` command, it is material independent and cannot be changed later. This is useful, for example, if you want to completely deactivate reemission for a neutral flux when defining the model, which can be achieved with a command such as:

```
add_neutral_flux model=my_model name=N sticking=1
```

Note:

The definition of a neutral flux does not include the specification of its angular distribution. The distribution of a neutral flux is isotropic by default, and you can set it by using the `define_nad` command (see [define_nad on page 290](#)).

The command `add_ion_flux` allows you to select the physical effects to take into account. For example, the following command defines an energy-independent ion flux called `I` for the model `my_model` with sputtering and reflection activated, and sputter deposition deactivated:

```
add_ion_flux model=my_model name=I energy=independent \
    reflection=true sputter_deposition=false sputtering=true
```

Note:

The definition of an ion flux does not include the specification of its angular distribution, which is provided using the `define_iad` command.

Specifying User-Defined Parameters

In this step, you specify user-defined parameters. Here, their attributes (for example, name, valid range, and default value) are set without assigning the actual values of the parameters.

User-defined parameters can be floating-point or integer values, and they are introduced using the `add_float_parameter` and `add_int_parameter` commands, respectively.

In addition, user-defined parameters can be either material dependent or global (material independent). If a parameter is material dependent, it can be assigned a different value for each material. Since deposition uses only one material, material-dependent parameters can be used only in the rate formulas of the `etch` and `etchdepo` models. A default value must be specified for material-dependent parameters. This value is used for materials that are present in the structure but have not been configured in the machine using the `add_material` command.

For example, a material-dependent floating-point parameter named `p`, with default value equal to 5, valid range from 3 to 7, and representing a velocity, can be introduced using the command:

```
add_float_parameter name=p model=my_model min=3 max=7 default=5 \
    quantity=velocity scope=material_dependent
```

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Model Definition

As previously mentioned, the actual values of the parameters are not set here, but when you configure a machine using the model to which the parameters belong. The values of the global parameters are set with the `define_etch_machine` or `define_deposit_machine` command; whereas, the values of the material-dependent parameters are set with the `add_material` command.

Defining a Rate Formula

The rate formula is defined with the `expression` parameter of the `add_formula` command.

Such an expression might involve any user-defined parameter, and the direct and indirect fluxes of any neutral and ion fluxes, as well as built-in functions to access properties of the exposed surface and mathematical functions.

User-defined parameters can be used in the expression by using their names followed by parentheses () .

The values of the direct and indirect fluxes can be obtained in the rate formula by the RFM built-in functions listed in [Data Available for Rate Calculation on page 574](#).

For example, if a neutral flux `N`, an ion flux `I`, and the parameters `p1`, `p2`, `p3`, and `p4` have been introduced in the model `my_model`, the following statement is a rate formula definition:

```
add_formula model=my_model expression="p1() * total_flux(N) + \
p2() * cos(theta()) - p3() * direct_flux(I) - p4() * sputtered_flux(I)"
```

Note:

In the rate formula, positive rates correspond to deposition, and negative rates correspond to etching.

Sentaurus Topography 3D also supports material-dependent rate formulas. This means that the mathematical expression used to compute the rate can be different for different materials. A rate formula for a specific material can be specified with the `material` parameter.

For example, the following commands define one rate formula specific for silicon, one specific for photoresist, and one used for all the other materials:

```
add_formula model=my_model material=Silicon \
expression="-p3() * total_flux(I)"

add_formula model=my_model material=Photoresist \
expression="-p2() * cos(theta())"

add_formula model=my_model expression="-p1() * total_flux(N)"
```

Machine Configuration

After the definition of a new model, you set up a machine that uses the newly defined model. This is very similar to setting up a machine using a built-in or a PMI model. However, the specification of model parameters related to ion or neutral fluxes must be performed with separate commands because an RFM model can use an arbitrary number of fluxes, and the reflection and yield functions must be configured separately.

Configuring a Machine

The configuration of a machine based on an RFM model consists of the following steps:

1. [Defining a Machine and Specifying User-Defined Global Parameters](#)
2. [Specifying Flux Parameter Values on page 570](#)
3. [Specifying User-Defined Material-Dependent Parameter Values on page 571](#)

Defining a Machine and Specifying User-Defined Global Parameters

Use the `define_etch_machine` command to configure a machine for models defined with `type=etch` or `type=etchdepo`. Use the `define_deposit_machine` command to configure a machine for models defined with `type=deposit`.

The configuration of a machine with an RFM model requires the following additional information:

- The name of the RFM model must be specified with the `model` parameter.
- If the model is a `deposit` model, then the material to deposit must be specified with the `material` parameter.
- If the model is an `etchdepo` model, then the material to deposit must be specified with the `deposit_material` parameter.
- If neutral fluxes are involved in the model, then the name of a collection of neutral distributions, containing the distributions of all the neutral fluxes of the model, can be specified with the `nad` parameter. Otherwise, all neutral fluxes will be assumed to have an isotropic distribution.
- If ion fluxes are involved in the model, then the name of a collection of ion distributions containing the distributions of all the ion fluxes of the model must be specified with the `iad` parameter.
- If sputtering is activated for at least one ion flux of the model, then the name of a collection of yield functions must be specified with the `yield` parameter. This collection

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Machine Configuration

must contain a yield function for all combinations of ion fluxes for which sputtering is activated and all materials that appear on the surface during at least one of the time steps.

- If reflection is activated for at least one ion flux of the model, then the name of a collection of reflection functions must be specified with the `reflection` parameter. This collection must contain a reflection function for all combinations of ion fluxes for which reflection is activated and all materials that appear on the surface during at least one of the time steps.
- The values of all the global parameters that are not optional, that is, those defined with `optional=false`.

Note:

The specified collection of reflection or yield functions does not have to contain functions for materials that are present in the structure but do not appear at the surface in any of the time steps.

For example, if `my_model` is an etch RFM model with ion fluxes having sputtering activated and it involves a mandatory global parameter `p`, a machine using such a model can be defined with the command:

```
define_etch_machine model=my_model iad=my_iad yield=my_yield p=0.5
```

If the parameter `p` is defined with `optional=true`, this parameter can be omitted from the `define_etch_machine` command.

Specifying Flux Parameter Values

The values of the parameters required to compute the indirect fluxes involved in the model are set using the `add_flux_properties` command.

For neutral fluxes, the sticking coefficient can be set with this command. For ion fluxes with sputter deposition activated, the sticking coefficient, the sputter type, and the sputter exponent can be set with this command.

For `etch` and `etchdepo` models, the flux parameters must be material dependent; whereas, for `deposit` models, they must be material independent.

Note:

The set of flux parameters is not defined by users, but it is determined by the fluxes involved in the model and by the physical effects activated for them. For example, the following command sets the sticking coefficient for the neutral flux `N` of a `deposit` model to 0.4:

```
add_flux_properties flux=N sticking=0.4
```

Specifying User-Defined Material-Dependent Parameter Values

The values of global parameters are set by the `define_etch_machine` or `define_deposit_machine` command; whereas, the values of material-dependent parameters are set by the `add_material` command. Each `add_material` command sets the values of the material-dependent parameters for a certain material.

Only the values of the material-dependent parameters defined with `optional=false` must be set in the `add_material` command. If a parameter is defined with `optional=true`, the specification of its value is optional in any `add_material` command, and its default value is used for all materials for which it has been omitted.

Therefore, the default value of a material-dependent parameter is used in two different cases:

- When no `add_material` command is issued for a certain material
- When a material-dependent parameter is defined as optional (`optional=true`) and it is omitted in an `add_material` command

Note:

It is not necessary to specify material properties with the command `add_material` for all materials, even if none of the material-dependent parameters is optional. All materials for which no properties have been specified explicitly with the command `add_material` are treated equally by using the default values of the material-dependent parameters.

For example, assume that two material-dependent parameters, `p1` and `p2`, are defined as follows:

```
add_float_parameter name=p1 scope=material_dependent default=0.1 \
    optional=true ...

add_float_parameter name=p2 scope=material_dependent default=0.5 \
    optional=false ...
```

In addition, suppose that `p1` and `p2` are the only material-dependent parameters involved in the model for which the machine is being configured. Accordingly, the following statements are valid:

```
add_material material=Silicon p1=0.3 p2=0.9

add_material material=Oxide p2=0.7
```

The first statement sets the values of all the material-dependent parameters. In the second statement, the specification of the value of the optional parameter is omitted and its default value 0.1 is used. For any other material, the default values 0.1 and 0.5 for the parameters `p1` and `p2`, respectively, will be used.

RFM Commands

The commands for the creation and use of RFM models are provided in [Chapter 6 on page 137](#). The commands for creating RFM models are listed approximately in the order in which they are used:

- `define_model`
- `add_neutral_flux`
- `add_ion_flux`
- `add_float_parameter`
- `add_int_parameter`
- `add_formula`
- `finalize_model`

The commands for using RFM models are:

- `define_deposit_machine`
- `define_etch_machine`
- `add_flux_properties`

Rate Calculation

The rate formulas defined with the `add_formula` command are used to calculate the deposition or etching rate for each surface element (see [add_formula on page 164](#)):

- For deposition, the rate must be greater than or equal to zero.
- For etching, the rate must be less than or equal to zero.
- For simultaneous etching and deposition, there is no restriction on the values of the rate; deposition is represented by positive values and etching by negative values.

Syntax for Formulas and Subexpressions

The syntax for formulas and subexpressions consists of the following components:

- Numeric constants
- Arithmetic operators: +, -, *, /

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Rate Calculation

- Mathematical constants: `e()`, `pi()`
- Mathematical functions: `abs(x)`, `sin(x)`, `cos(x)`, `tan(x)`, `asin(x)`, `acos(x)`, `atan(x)`, `atan2(x, y)`, `sinh(x)`, `cosh(x)`, `tanh(x)`, `exp(x)`, `log(x)`, `log10(x)`, `pow(x, y)`, `sqrt(x)`, `ceil(x)`, `floor(x)`
- Conditional and relational functions: `checked_div(x, y)`, `checked_div(x, y, z)`, `high_pass(x, y, z)`, `higher_pass(x, y, z)`, `low_pass(x, y, z)`, `lower_pass(x, y, z)`, `max(x, y)`, `min(x, y)`
- Parentheses
- Data access functions described in [Data Available for Rate Calculation on page 574](#)
- Subexpressions previously defined with the `subexpression` parameter of the `add_formula` command

The arguments `x`, `y`, and `z` to these functions are themselves expressions.

Conditional and Relational Functions

The following functions are available to implement conditions and control flow:

- `checked_div(<numerator>, <denominator>)`
Returns `numerator / denominator` if `denominator != 0`.
Otherwise, returns `numerator`, that is, it is equivalent to
`checked_div(<numerator>, <denominator>, <numerator>)`.
- `checked_div(<numerator>, <denominator>, <replacement>)`
Returns `numerator / denominator` if `denominator != 0`.
Otherwise, returns `replacement`.
- `high_pass(<expression>, <threshold>, <attenuation>)`
Returns `expression` if `expression >= threshold`. Otherwise, returns `attenuation`.
- `higher_pass(<expression>, <threshold>, <attenuation>)`
Returns `expression` if `expression > threshold`. Otherwise, returns `attenuation`.
- `low_pass(<expression>, <threshold>, <attenuation>)`
Returns `expression` if `expression <= threshold`. Otherwise, returns `attenuation`.
- `lower_pass(<expression>, <threshold>, <attenuation>)`
Returns `expression` if `expression < threshold`. Otherwise, returns `attenuation`.
- `min(<left>, <right>)`
Returns `left` if `left <= right`. Otherwise, returns `right`.
- `max(<left>, <right>)`
Returns `left` if `left >= right`. Otherwise, returns `right`.

Data Available for Rate Calculation

The following functions are available to access data related to a surface element, which is available for use in the formula for a deposition or an etching rate:

- `defined_yield(<flux>)`: Returns the value of the yield function for the specified ion flux and the material of the current surface element, and the angle between the vertical and the surface normal of the current element. This function is available for all ion fluxes and the `default_species`.

Note:

Models using this function in any of their rate formulas are not supported by a machine having `rotation=continuous`. In models to be used with machines having `rotation=continuous`, the sputtered flux can be computed using the function `sputtered_flux(<flux>)`.

- `defined_yield(<flux>, <material>)`: Returns the value of the yield function for the specified ion flux and the specified material, and the angle between the vertical and the surface normal of the current element. This function is available for all ion fluxes and the `default_species`.

Note:

Models using this function in any of their rate formulas are not supported by a machine having `rotation=continuous`. In models to be used with machines having `rotation=continuous`, the sputtered flux can be computed using the function `sputtered_flux(<flux>)`.

- `direct_flux(<flux>)`: Returns the value of the direct flux arriving at the surface element for the specified flux (all neutral and ion fluxes).
- `directional_value(<value_100>, <value_110>, <value_111>)`: The first argument specifies the value for the `<100>` direction; the second argument, the `<110>` direction; and the third argument, the `<111>` direction. Depending on the direction of the surface normal of an element, an interpolated value is calculated and returned. This function can be used to implement orientation-dependent etching or deposition models.
- `is_void()`: Returns 1 if the surface element belongs to a void boundary; 0 otherwise.
- `pad_pressure()`: Returns the pressure produced by the pad at the surface element in Pa.

Note:

The following limitations apply:

- Only models of type equal to `etch` or `etchdepo` support this function in their rate formula expressions.

Chapter 8: Rate Formula Module

Rate Calculation

- Models using this function cannot use these RFM functions:
`direct_flux(<flux>), sputter_depo_flux(<flux>),
sputtered_flux(<flux>), total_flux(<flux>).`
- Periodic boundary conditions are used to evaluate the RFM function
`pad_pressure()` independently of what has been specified with the command
`define_boundary_conditions`.
- `<parameter>()`: Returns the value of the specified global or material-dependent user-defined parameter.
- `sputter_depo_flux(<flux>)`: Returns the value of the flux of the redeposited sputtered material associated with the specified ion flux arriving at the surface element (ion flux with sputter deposition activated).
- `sputtered_flux(<flux>)`: Returns the value of the sputter flux emitted from the surface element for the specified ion flux (ion flux with sputtering activated).
- `sticking(<flux>)`: Returns the value of the sticking parameter that was specified with the `add_flux_properties` command for the given flux (neutral flux or ion flux with sputter deposition activated).
- `<subexpression>()`: Returns the value of the specified subexpression. If the current expression is global, only other global subexpressions can be accessed. If the current expression is material dependent, other subexpressions for the same material or global subexpressions can be accessed.
- `theta()`: Returns the value of the angle between the surface normal and the vertical. The value is in the range $[0, \pi]$.

Note:

Models using this function in any of their rate formulas are not supported by a machine having `rotation=continuous`.

- `total_flux(<flux>)`: Returns the value of the total flux arriving at the surface element for the specified flux (neutral flux or ion flux with reflection activated).
- The total integrated ion flux is defined as $\Gamma_{\text{total}}^{\text{ion}} = \Gamma_{\text{direct}}^{\text{ion}} - \Gamma_{\text{direct reflected}}^{\text{ion}} + \Gamma_{\text{reflection}}^{\text{ion}}$ where:
 - $\Gamma_{\text{direct reflected}}^{\text{ion}}$ is the portion of the direct flux that has been reflected away from a surface element.
 - $\Gamma_{\text{reflection}}^{\text{ion}}$ is the sum of all fluxes incoming at a surface element that were reflected from other surface elements.
- `visible()`: Returns if the surface element is visible from vertically above. Returns 1 if the surface element is visible or 0 otherwise.

Chapter 8: Rate Formula Module

Rate Calculation

Models using the `visible()` function in any of their rate formulas are not supported by a machine having `rotation=continuous`.

Note:

A syntax error occurs if functions taking a flux name as argument are used with a flux that is of an incompatible type.

The identifier `default_species` can be used as a placeholder parameter for the `defined_yield` functions in models that do not specify any ion fluxes to access yield functions. The yield functions must be defined with `default_species` as the species.

The integrated direct reflected flux and the reflection flux are not accessible as RFM functions. However, they are available as datasets created when using the `plot_interval` parameter of the `deposit` and `etch` commands.

Examples

The `direct_flux()` function is available to a model with only a neutral flux `n`. However, the `sputtered_flux()` function is not available:

```
define_model name=N type=deposit description=""  
  
add_neutral_flux model=N name=n  
  
# Next command causes a syntax error because n is not a valid argument  
# for sputtered_flux().  
add_formula model=N expression={direct_flux(n) + sputtered_flux(n)}  
  
finalize_model model=N
```

Similarly, if ion fluxes are defined for a model but the necessary effects are deactivated, a syntax error occurs:

```
define_model name=I type=deposit description=""  
  
add_ion_flux model=I name=i energy=independent reflection=false \  
    sputtering=true sputter_deposition=false  
  
# Next command causes a syntax error because i is not a valid argument  
# for sputter_depo_flux().  
add_formula model=I expression={direct_flux(i) + sputter_depo_flux(i)}  
  
finalize_model model=I
```

Chapter 8: Rate Formula Module

Example: Reimplementing and Using ionmill Etching Model

Example: Reimplementing and Using ionmill Etching Model

The following example demonstrates how the `ionmill` etching model can be reimplemented and used as an RFM model:

```
define_model name=mck_ionmill type=etch \
    description="user-defined ionmill etching"

add_float_parameter model=mck_ionmill name=rate min=0 default=0 \
    scope=material_dependent quantity=velocity

add_float_parameter model=mck_ionmill name=s1 default=1 \
    scope=material_dependent quantity=dimensionless

add_float_parameter model=mck_ionmill name=s2 default=0 \
    scope=material_dependent quantity=dimensionless

add_formula model=mck_ionmill \
    expression={ -rate() * visible() * (s1() * cos(theta()) \
    + s2() * pow(cos(theta()), 2) \
    + (1 - s1() - s2()) * pow(cos(theta()), 4)) }

finalize_model model=mck_ionmill

define_etch_machine model=mck_ionmill

add_material material=Silicon rate=0.9 s1=5.5 s2=-6

add_material material=Oxide rate=0.7 s1=5 s2=-7

etch ...
```

References

- [1] T. K. Chini *et al.*, “The angular dependence of sputtering yields of Ge and Ag,” *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, vol. 72, no. 3–4, pp. 355–358, 1992.

9

Working With Reaction Models

This chapter explains how to use reaction models based on the particle Monte Carlo (PMC) method. It also discusses how to integrate PMC-based simulations with other Sentaurus Topography 3D functionality.

Setting Up a Simulation Using a Reaction Model

This section provides a simple example to start using reaction models. A model for a simple process will be set up and a simulation using that model will be run.

In the process you want to model, fluorine gas is fed to the reactor, where a silicon wafer is being processed. When fluorine reaches silicon, they react with a given probability, and silicon is etched.

The first step is to define the model. A reaction model consists of:

- The source species, that is, the species coming from the reactor in a gaseous state
- The reactions relevant for the modeled process

A reaction model for the above-described process can be set up as follows:

```
# Begin the definition of a model named 'm1'.
define_model name=m1 description="Simple reaction model"

# Add a species named "F" coming from the reactor to model 'm1'.
add_source_species model=m1 name=F

# Add a reaction named 'etch_reaction' to model 'm1'.
# According to this reaction, when species 'F' and 'Silicon' react, a
# silicon atom is removed and a 'SiF' molecule goes into the reactor.
# The net effect is to remove a silicon atom from the structure.
add_reaction model=m1 name=etch_reaction \
    expression="F<g> + Silicon<s> = SiF<g>"

# End the definition of model 'm1'.
finalize_model model=m1
```

Chapter 9: Working With Reaction Models

Setting Up a Simulation Using a Reaction Model

As for RFM models, the definition of a new reaction model starts with the `define_model` command (see [define_model on page 289](#)) and ends with the `finalize_model` command (see [finalize_model on page 499](#)).

Since fluorine gas molecules are electrically neutral, their angular distribution is assumed to be isotropic. An angular distribution described by [Equation 5 on page 49](#) with m equal to 1 describes an isotropic distribution. Therefore, an isotropic angular distribution can be set up for species F with the following command (see [define_species_distribution on page 337](#)):

```
define_species_distribution name=my_distribution species=F \
    exponent=1 flux=1e-3
```

After the model and the distribution of its source species have been specified, a machine can be defined using the `define_etch_machine` command (see [Machines on page 29](#) and [define_etch_machine on page 242](#)):

```
define_etch_machine model=m1 name=m1_machine \
    species_distribution=my_distribution
```

In Sentaurus Topography 3D, machines are used to select the model to use for the simulation and to assign the parameter values required by the selected model. Reaction models require probabilities to be set for each reaction. The reaction probabilities specify the probability that a reaction will occur when its reactants become available.

The following `add_reaction_properties` command (see [add_reaction_properties on page 188](#)) sets the reaction probability to 0.7 for the reaction named `etch_reaction` of the model used by the machine named `m1_machine`:

```
add_reaction_properties machine=m1_machine reaction=etch_reaction p=0.7
```

The machine is now fully set up and can be used to process a structure. As explained in [Simulating Process Steps on 2D and 3D Structures on page 32](#), the initial structure can be either loaded from a TDR boundary file or defined using geometric etching and deposition steps. For simplicity, assume that the initial structure is stored in a TDR file called `init.tdr`. Then, the following two commands define the initial structure and start a simulation using the machine defined above, respectively:

```
define_structure file=init.tdr
etch spacing=0.1 time=0.5 method=pmc machine=m1_machine
```

The results of a simulation that used the PMC method can be saved in TDR file format with the command (see [save on page 521](#)):

```
save type=gc
```

Integration With Other Sentaurus Topography 3D Functionality

The `etch` command runs a simulation using the selected machine. The name of the resulting structure is specified by the parameter `structure` of the `etch` command.

The data structure used to store internally the result depends on the simulation method used (see [Sentaurus Topography 3D Computational Model on page 23](#) and parameter `method` of `etch` on page 399):

- When `method=levelset`, when etching with a mask or etching a geometric shape, the simulation result is stored internally in a boundary data structure (see [Boundary Types on page 31](#)).
- When `method=pmc`, the simulation result is stored internally in a volumetric data structure.

Table 86 Commands requiring input structures to be stored internally in a boundary data structure

Command	Comment
<code>deposit</code>	
<code>etch</code>	When using a level set-based model or when etching a geometric shape or a mask.
<code>extend_structure</code>	
<code>extract</code>	See Table 66 on page 465 .
<code>fill</code>	
<code>filter_structure</code>	See Table 69 on page 486 .
<code>litho</code>	
<code>pattern</code>	
<code>save</code>	When <code>type=closed_surface</code> , or <code>type=exposed_surface</code> , or <code>type=final_structure</code> . Note: When <code>type=gc</code> , <code>type=pmc</code> , <code>type=transfer</code> , <code>type=vbe</code> , or <code>type=volume_fractions</code> is specified, the <code>save</code> command requires the input structure to be stored in a <i>volumetric</i> data structure.
<code>truncate</code>	

Converting a Result Structure to TDR Boundary File Format

Whenever any of the commands in [Table 86](#) must be executed on the result of a simulation that used the PMC method, an explicit conversion is needed.

You can use the `filter_structure` command to convert the result of a PMC-based simulation to a structure stored in TDR boundary file format (see [filter_structure on page 483](#)), as demonstrated in the following example. In particular, the `filter_structure` command is used twice:

- Before starting the simulation using the PMC method, it creates a copy of the initial structure (`filter_structure type=copy`).
- When the simulation is completed, it runs Boolean operations (`filter_structure type=boolean`) and produces a structure stored in TDR boundary file format.

Example

```
# The 'define_structure' command creates a structure that is
# stored internally in TDR boundary file format. The newly
# created structure is named 'default_structure'.
define_structure material=Silicon point_min={0 0 0} point_max={1 1 1}

# The 'fill' command operates on a structure stored in TDR
# boundary file format. The result of the command 'fill'
# overwrites the structure named 'default_structure' and
# is still stored internally in TDR boundary file format.
fill material=Oxide thickness=0.5

# A shape named 's' is defined to create an opening in the oxide
# layer added with the command 'fill'.
define_shape type=cube name=s point_min={0.2 0.2 1} \
    point_max={0.8 0.8 2}

# The shape 's' is etched away from the structure named
# 'default_structure'. The result of the command 'etch'
# overwrites the structure 'default_structure' and is still
# stored internally in TDR boundary file format.
etch shape=s

# A copy of structure 'default_structure' is created. The copy
# is named 'initial_structure' and is stored in TDR boundary
# file format as well.
filter_structure type=copy name=initial_structure

# A reaction model named 'reaction_model' is defined.
define_model name=reaction_model description=""
...
finalize_model model=reaction_model
...
```

Chapter 9: Working With Reaction Models

Integration With Other Sentaurus Topography 3D Functionality

```
# A machine using model 'reaction_model' is defined.  
define_etch_machine model=reaction_model ...  
...  
# The structure named 'default_structure' is etched using the  
# reaction model named 'reaction_model'. The result structure  
# overwrites the structure named 'default_structure'.  
# Since the PMC method was used, the result of this command  
# is stored internally with a volumetric data structure.  
etch spacing=0.1 time=1 method=pmc  
  
# The structure 'default_structure' stored in a volumetric  
# data structure is saved in the appropriate TDR file format  
# (see Table 86).  
save type=gc  
  
# A new structure named 'boundary_structure' is created using  
# a Boolean operation. The operands of the Boolean operation  
# are specified with the parameters 'body' and 'structure'. It  
# is worth noting that the structure given with the parameter  
# 'body' is stored internally in TDR boundary file format; whereas,  
# the structure given with parameter 'structure' is stored  
# internally in a volumetric data structure in TDR file format.  
filter_structure type=boolean body=initial_structure \  
    structure=default_structure name=boundary_structure  
  
# Since the structure named 'boundary_structure' is stored  
# in TDR boundary file format, the 'extract' command can be  
# used to return information on it (see Table 86).  
extract type=1d_cut structure=boundary_structure ...  
...  
  
# Since the structure named 'boundary_structure' is stored  
# in TDR boundary file format, it can be saved with  
# type=final_structure (see Table 86).  
save structure=boundary_structure type=final_structure
```

Boolean operations are not run automatically after each PMC-based simulation to convert the resulting structure into a boundary data structure because they are computationally expensive and are not always needed. Boolean operations are necessary only when one of the commands in [Table 86](#) must be run, but they are not required to save the resulting structure in a TDR file format and to visualize it. In addition, PMC-based simulations can be run on the result of a previous PMC-based simulation without executing any Boolean operations.

10

Physical Model Interface for Etching and Deposition

This chapter describes the physical model interface for etching and deposition.

The physical model interface (PMI) gives you the possibility to extend the modeling capabilities of Sentaurus Topography 3D by implementing a new model in the form of a C++ class. The PMI supports three different modes: deposition, etching, and simultaneous etching and deposition.

Sentaurus Topography 3D uses the level-set method to move the exposed surface during a time step. However, direct use of the level-set data structures requires detailed knowledge of the particular implementation and, therefore, direct use is complicated and error prone. An explicit surface representation is used for the PMI in Sentaurus Topography 3D.

The following sections describe the command file interface for using a PMI-based model, the C++ interface for creating a new model, and the input and output parameters.

Command File Interface

The `add_material`, `define_deposit_machine`, and `define_etch_machine` commands can handle PMI-based models.

The name with which a PMI-based model is specified, with the `model` parameter of the `define_deposit_machine` and `define_etch_machine` commands, is defined in the source code of the model and can have an arbitrary value. The only restriction is that it must not be identical to the name of a built-in model.

Note:

Model names beginning with the prefix `pmi` are guaranteed not to conflict with built-in models.

In the command file, the parameters of a PMI-based model are specified in the same way as for built-in models. Therefore, for deposition models, all model parameters are specified using the `define_deposit_machine` command. For etching models, the

Chapter 10: Physical Model Interface for Etching and Deposition

C++ Interface

material-independent parameters of the model are specified with the `define_etch_machine` and the material-dependent parameters with the `add_material` command. For simultaneous etching and deposition, the deposition-specific parameters are specified with the `define_etch_machine` command.

A PMI-based model can have an arbitrary number of model-specific command file parameters. These parameters can have arbitrary names. The only restriction on the parameter names is that they must not be identical to the names of built-in parameters of a PMI-based model.

[Table 87](#) lists the built-in parameters of the PMI-related commands. The command file parameters have four possible types: Boolean, floating point, integer, and string.

Table 87 Built-in parameters of commands for using PMI-based models

Command	Built-in parameters
<code>add_material</code>	<code>machine, material</code>
<code>define_deposit_machine</code>	<code>material, model, name, rotation, tilt</code>
<code>define_etch_machine</code>	<code>deposit_material, model, name, rotation, tilt</code>

A default value must be specified for each user-defined parameter, and you can specify whether a user-defined parameter is optional or mandatory. When specifying the parameters for a material with the `add_material` command, a parameter can be omitted if it has been declared as optional. In this case, the default value will be used.

Depending on the type of a parameter, the default value can be queried directly with the `bool_parameter_default()`, `float_parameter_default()`, `int_parameter_default()`, or `string_parameter_default()` function.

C++ Interface

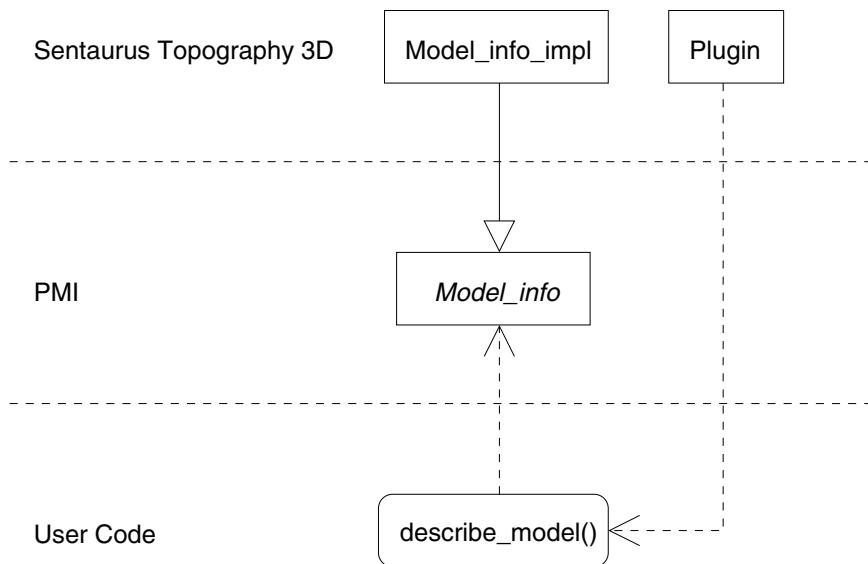
At the C++ level, the interface consists of several abstract base classes:

- `Model_info` defines the model name, the model-specific command file parameters, and the plot datasets generated by the model.
- `Model_rate` calculates the surface rate and the plot datasets for each time step.
- `Global_data` provides access to the values of the command file parameters and other data that does not change during the time steps.
- `Time_step_data` provides access to surface-related data and data that changes between time steps.

The developer of a PMI-based model must implement a class that is derived from `Model_rate` and must implement three free functions.

The function `describe_model()`, which must be implemented by users, is called during the initialization of a PMI-based model. It defines the model name, the model parameters, and the plot datasets generated by the model. [Figure 36](#) shows a unified modeling language (UML) diagram of the classes used to initialize a PMI-based model.

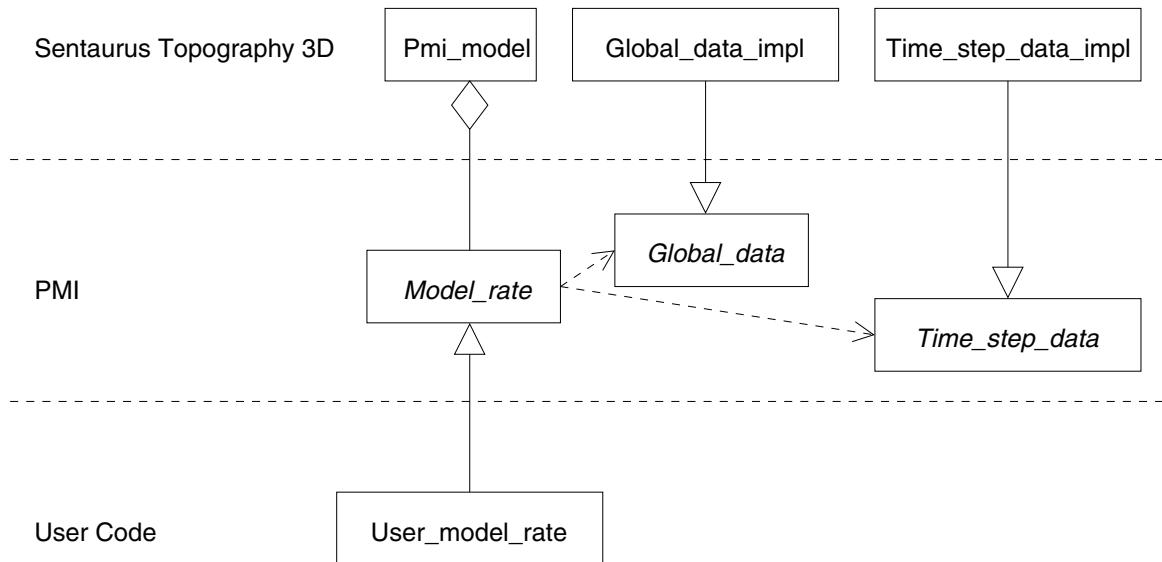
Figure 36 UML diagram for initializing a PMI model



The class derived from `Model_rate` is used in each time step to calculate the surface rate and to initialize the plot datasets. [Figure 37](#) shows a UML diagram of the PMI-related classes used for the surface rate calculation in each time step.

Detailed documentation of the abstract classes is available in the corresponding header files, which are located in the directory `${STROOT} /tcad/${STRELEASE}/lib/sptopo3d/include`.

Figure 37 PMI class hierarchy for calculating surface rates



Implementing a New Model

As previously mentioned, to implement a PMI-based model, it is necessary to implement the function `describe_model()`. The only argument of this function is a reference to an object derived from `Model_info`. This object is used to define the model name and whether the model is used for deposition, or etching, or simultaneous etching and deposition. Besides that, it is used to define all model-specific command file parameters (name, type, and default value if applicable), and the names and units of the datasets that are generated by the model.

A class derived from `Model_rate` is used to implement the surface rate calculation for each time step. An instance of the class derived from `Model_rate` is created when the `deposit` or `etch` command is executed. For each time step, the function `Model_rate::calculate_rate()` is called to calculate the surface rates and the plot datasets. The free functions `model_rate_factory()` and `model_rate_delete()` are used to create and delete instances of the class derived from `Model_rate`, respectively.

Information Available to a Model

All input data available to a PMI-based model is provided by the classes `Global_data` and `Time_step_data`.

The class `Global_data` makes the values of model-specific command file parameters available. In addition, it contains the names of all the materials of the input structure and

other data that does not change between time steps. For example, for etching models, a list of all materials for which parameters have been defined with the `add_material` command is available.

The class `Time_step_data` provides information about the current surface and its properties. It also contains other data that changes between time steps, for example, the size of the previous time step.

For each surface vertex, a list of indices in the list of structure materials at the vertex is available. If the vertex is located at a material interface, the list of structure material indices will contain more than one entry, and you are responsible for choosing which material will be used for the rate calculation.

Information about the surface material is available in all three modes. This information allows models to calculate material-specific rates also for the deposition mode.

The arguments of the free function `model_rate_factory()` are a reference to an object derived from `Global_data` and a reference to an object derived from `Time_step_data`. Therefore, all information is available to the constructor of the class derived from `Model_rate`, which is called in `model_rate_factory()`. The reference to the object derived from `Global_data` is guaranteed to be valid for the entire lifetime of the PMI model instance.

In `Model_rate::calculate_rate()`, a reference to an object derived from `Time_step_data` is available. In addition, you obtain a reference to an object derived from `Plot_data`, which provides access to the plot data arrays.

Additional Input Data

Additional input data that is too complicated to be read from the command file might be required by a model, for example, complex chemical reactions. This kind of data can be read and stored as member data by the constructor of the derived class for later use in `Model_rate::calculate_rate()`.

In some models, it might be necessary to store data from previous time steps. This additional data also can be stored as member data of the derived class object.

Data Types Used in Interface

To avoid linking problems, only C-style data types or types for which the corresponding header files are provided are used in the interface. While this makes handling the data more cumbersome, it helps to prevent problems that are difficult to debug.

Error Handling

The only safe way to signal to the calling code that an error has occurred in a constructor is to throw an exception. However, C++ does not allow exceptions to cross interfaces as they are used for the PMI.

An exception that is thrown in a PMI model and that is not caught and handled in the PMI model will terminate the simulation immediately. For a PMI model, this means that exceptions that were thrown in the constructor must be caught in the factory functions. If there is an error, the null pointer is returned and the simulation is stopped in a controlled way.

Similarly, exceptions must not leave `Model_rate::calculate_rate()`. Here, an error is signaled to the calling code by returning the value `false`. The simulation is then stopped in a controlled way.

The function `Global_data::message()` can be used to output messages to the standard output and the log file. For error messages, the verbosity level should be set to low; while for other messages, a verbosity level of medium or higher should be used.

Compiling the Source Code

The source code can be compiled and linked using the `cmi` tool, which calls the C++ compiler and linker with the correct command-line options for each supported platform.

The `cmi` tool is contained in each TCAD release and is mainly used for Sentaurus Device CMI-based and PMI-based models:

```
cmi -I${STROOT}/tcad/${STRELEASE}/lib/sptopo3d/include User_model_rate.cc
```

See *Compact Models User Guide*, Compilation of C++ (.C) Files.

Using Additional Source Files or Libraries

A PMI-based model is not limited to the functionality declared in the abstract base classes of the PMI or directly derived from it. You can use additional source files or libraries, which provide additional functionality, to build the shared library for a model. For example, a model might need to solve a linear equation system. In this case, it is possible to link with a library that provides this functionality.

Additional source files or libraries can be specified as command-line parameters for the `cmi` tool, which will combine them into one shared library.

Using the C++ Standard Library

When using the features of the C++ Standard Library in the implementation of a PMI-based model, depending on the platform, it might be necessary to link an additional library that provides this functionality. For example, on 64-bit Linux, it is necessary to link `libstdc++` by adding `-lstdc++` to the command-line parameters of the `cmi` tool.

To avoid problems at link-time or runtime, it is necessary to use *exactly* the same version of the C++ compiler for the compilation of the PMI code as used for the compilation of Sentaurus Topography 3D.

See *Compilers for CMI and PMI* in the TCAD Sentaurus release notes for information about the compiler versions used in Sentaurus Topography 3D.

Loading the Shared Library

During initialization of the simulator, the current directory and the path defined with the environment variable `SPTOPO3D_PMI_PATH` are searched for shared libraries that conform to the CMI-naming or PMI-naming convention (platform-specific suffix, for example `.so.linux64`).

These files are loaded and searched for the three free functions: `describe_model()`, `model_rate_factory()`, and `model_rate_delete()`. If all three functions are found, the model is added to the list of available models and can then be used for an arbitrary number of deposition or etching steps. Otherwise, the shared library is closed again.

Note:

The shared library containing a PMI model is unloaded only when the simulator is stopped. This must be taken into account when using static variables.

Debugging

Debugging the PMI code is more difficult than debugging a standard program for several reasons:

- Only the PMI code created by users is available as source code, and debugging symbols are not available for Sentaurus Topography 3D.
- The library containing the PMI code is loaded dynamically whenever the conditions mentioned in the previous section are fulfilled.
- Typically, Sentaurus Topography 3D is started by a wrapper script that sets some environment variables. When using a debugger, it is necessary to set these environment variables manually and then to start the debugger with the executable of Sentaurus Topography 3D without the wrapper script.

Chapter 10: Physical Model Interface for Etching and Deposition

Input and Output Parameters

The details of debugging are highly platform dependent and tool dependent, especially when using shared libraries.

Input and Output Parameters

This section describes the input parameters available to a PMI-based model.

The following input data is available from objects derived from `Global_data`, `Time_step_data`, and `Plot_data` for model initialization and rate calculation:

- Model-specific command file parameters
- Default values of model-specific command file parameters
- Model-specific plot datasets
- Surface vertices
- Surface normal at vertices
- Curvature at vertices
- Area associated with surface vertices
- Material at vertices
- Mutual visibility between surface vertices
- Point classification (inside, on surface, outside)
- Size of the previous time step
- Machine materials
- Structure materials
- Conversion between material indices and material names
- Conversion between material names and material indices
- Direct flux at vertices for analytic flux distributions
- Visibility of vertices from source vertically above
- Neighbor elements information

The output parameter for the rate calculation is an array containing the rate at each surface vertex.

Chapter 10: Physical Model Interface for Etching and Deposition

Input and Output Parameters

Each surface vertex belongs to a discretization element of the surface. For each surface vertex, information about the neighbor elements is available.

The `Plot_data` parameter provides access to the plot datasets and to a query function that determines whether plotting is activated.

11

Known Issues and Limitations

This chapter provides information about issues and limitations in the use of Sentaurus Topography 3D.

This chapter covers the following topics:

- [Issues Applicable to the Level-Set Method](#)
- [Issues Applicable to the Particle Monte Carlo Method](#)
- [Other Issues](#)

Issues Applicable to the Level-Set Method

The following issues and limitations apply to the level-set method:

- There is no support for energy-dependent flux integration in level set-based models.
- As described in [Discretization Size and Accuracy When Using the Level-Set Method on page 27](#), using the level-set method to discretize and move the surface of a structure introduces artifacts. When using models for simultaneous etching and deposition, these artifacts can cause the creation of thin layers of deposited material. Depending on the values of the model parameters, this might prevent etching and cause even more deposition.
- When using a machine having `model=crystal`, the `deposit` command does not support the `cfl`, `compute_first_plot`, `compute_last_plot`, `extraction_interval`, `extraction_times`, `extraction_times_unit`, `file`, `merge`, `plot_interval`, `plot_times`, `plot_times_unit`, `plot_type`, `stop_plane`, `stop_point`, and `update_scheme` parameters.
- When using a machine having `model=crystal`, the `etch` command does not support the `abs_min_deposition_thickness`, `cfl`, `compute_first_plot`, `compute_last_plot`, `extraction_interval`, `extraction_times`, `extraction_times_unit`, `file`, `min_deposition_thickness`, `plot_interval`, `plot_times`, `plot_times_unit`,

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Issues Applicable to the Level-Set Method

`plot_type`, `region_query_accuracy`, `stop_plane`, `stop_point`, and `update_scheme` parameters.

- When using a built-in model, the `add_interface_layer` command is not supported for the sticking and reflection parameters.

Two-Dimensional Structures

The following issues and limitations apply to the level-set method with regard to 2D structures:

- Reflective sputtering is not supported when processing 2D structures.
- Flux integration in two dimensions is performed with the radiosity method exclusively. There is no Monte Carlo engine in two dimensions.
- The `etch` command does not support the `mask` parameter for 2D structures.
- The `pattern` command is not available for 2D structures.

Rate Formula Module

The following issues and limitations apply to the level-set method with regard to the rate formula module (RFM):

- Reflection is not supported for the RFM when processing 2D structures.
- Boundary conditions set with the `define_boundary_conditions` command are ignored when using RFM models that use the RFM function `pad_pressure()` and periodic boundary conditions are always applied.
- Models using the RFM function `pad_pressure()` cannot use these RFM functions: `direct_flux(<flux>)`, `sputter_depo_flux(<flux>)`, `sputtered_flux(<flux>)`, `total_flux(<flux>)`.

Boundary Conditions, Tilt, and Rotation

The following issues and limitations apply to the level-set method with regard to boundary conditions, tilt, and rotation:

- Boundary conditions specified by the command `define_boundary_conditions` have no effect on the indirect flux computations for 2D structures.
- Only reflective boundary conditions are supported when using the built-in electrodeposition, `spin_on`, or wet deposition model.

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Issues Applicable to the Particle Monte Carlo Method

- The `define_boundary_conditions` command has no effect on the built-in deposition and etching models named `crystal`. Boundary conditions are always `reflective` in simulations using deposition and etching machines having `model=crystal`.
- Built-in models do not support machines with `rotation=continuous`.
- The RFM functions `defined_yield(<flux>)`, `defined_yield(<flux, material>)`, `theta()`, and `visible()` are not supported by etching or deposition machines with `rotation=continuous`.
- The radiosity method does not provide accurate results for machines with a tilt angle greater than approximately 70° for 3D structures. Use the Monte Carlo method for such machines.
- The `define_deposit_machine` command does not support the parameters `tilt` and `rotation` when `model=electrodeposition` or `model=spin_on`.
- The `define_etch_machine` command does not support the parameters `tilt` and `rotation` when `model=wet`.
- The `define_deposit_machine` and `define_etch_machine` commands do not support the parameters `tilt` and `rotation` when `model=crystal`.
- The parameters `tilt` and `rotation` of the `define_deposit_machine` and `define_etch_machine` commands do not support the radian measurement unit.

Issues Applicable to the Particle Monte Carlo Method

The following issues and limitations apply to the particle Monte Carlo (PMC) method:

- The parameter `structure` of the following commands cannot specify a PMC structure:
 - `deposit` (when using a level set-based model)
 - `etch` (when using a level set-based model)
 - `filter_structure` (`when type=convert_to_pmc, type=decimate, type=merge_regions, type=rediscretize_boundary, type=remove_disconnected_top_parts, type=remove_region, type=rename_region, type=replace_material, or type=smooth`)
 - `litho`
 - `save` (`when type=closed_surface, or type=exposed_surface, or type=final_structure`)

[Integration With Other Sentaurus Topography 3D Functionality on page 580](#) explains how to convert the structure in such a way that these commands can be used.

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Issues Applicable to the Particle Monte Carlo Method

- When `type=gc`, `type=pmc`, `type=vbe`, or `type=volume_fractions`, the parameter structure of the `save` command must specify a structure obtained as the result of a PMC-based simulation.
- The `flat_orientation` and `vertical_orientation` parameters of the `etch` command are not supported when `method=pmc`.
- Nonuniform spacing of the simulation grid is not supported when using the `etch` command with `method=pmc`.
- When using the `etch method=pmc` command to process a structure obtained as the result of a previous PMC-based simulation, the spacing specified with the `spacing` parameter is ignored.
- When running a simulation with a machine using a reaction model that allows deposition, the vertical extent of the computational domain must be large enough to contain the deposited material.
- The parameter structure of the `extract` command can specify a PMC structure only in any of the following cases:
 - When `type=bounding_box`, `type=dimension`, or `type=interface` is used to extract the interface between two materials (that is, when also parameters `material1` and `material2` are specified)
 - When `type=material_names` and `exposed_only=false`
 - When `type=probe` and `property=material`
 - When `type=probe` and `property=length`
- The parameter `stop_material` of the `etch` command can be used only when `method=pmc`.
- The parameter `compute_process_graph` is not supported when the `noise_reduction` parameter is set to a value other than 0.
- When you start Sentaurus Topography 3D with the `--processes` command-line option with a value greater than 1 (see [Table 1 on page 18](#)):
 - The parameter structure of the following commands must not denote a structure obtained from the command `etch method=pmc averaging_runs=1`:

```
etch method=levelset
etch mask=<c>
etch shape=<c>
extend_structure, extract, fill
filter_structure (except when type=copy)
litho, pattern
save (except when type=gc)
truncate
```

Chapter 11: Known Issues and Limitations

Other Issues

- The parameters `extraction`, `plot_interval`, `plot_times`, `stop_material`, `stop_plane`, and `stop_point` of the command `etch method=pmc averaging_runs=1` are not supported.
- The parameter `compute_process_graph=true`, machines using the parameter `damage` or volumetric source species, and structures using periodic boundary conditions are not supported by the command `etch method=pmc averaging_runs=1`.

Boundary Conditions, Tilt, and Rotation

The following issues and limitations apply to the PMC method with regard to boundary conditions, tilt, and rotation:

- When defining a machine that uses a reaction model, `rotation=continuous` can be used only if no source species of the reaction model has an energy-dependent distribution computed by the HPEM simulator, the Benoit-Cattin plasma sheath model, or the Edelberg–Aydil plasma sheath model, or imported from an energy angular distribution (EAD) file.
- Boundary conditions of type `none` are not supported when processing a structure with the PMC method.

Other Issues

The following issues and limitations apply to the level-set method and the PMC method:

- Sentaurus Lithography integration works only in three dimensions.
- The `add_litho_command`, `define_litho_machine`, and `litho` commands cannot be used when you start Sentaurus Topography 3D with a value greater than 1 for the command-line option `--processes` (see [From the Command Line on page 17](#)).
- The `slice_angle` parameter of the `define_structure` command does not support the radian measurement unit.
- The `filter_structure` command with `type=convert_to_pmc`, `type=smooth`, or `type=rediscretize_boundary` is not available for 2D structures.
- When `rotation=continuous` is used, the actual equivalent error for any species always approaches 0.5 as the tilt angle approaches 90°.

Chapter 11: Known Issues and Limitations

Other Issues

- The parameters `stop_plane`, `stop_point`, and `update_scheme` are not supported by the `deposit` command for machines having `model=spin_on`.
- For machines having `model=spin_on`, the `deposit` command does not support structures whose exposed surface cannot be described as a single-valued function of the x- and y-coordinates in three dimensions, or of the x-coordinate in two dimensions. However, topologically connected exposed surfaces are allowed to contain elements parallel to the vertical direction.

A

Examples

This appendix provides examples that demonstrate how to use different Sentaurus Topography 3D models.

Three-dimensional input structures can be created using either Sentaurus Topography 3D itself or Sentaurus Structure Editor. Examples of how to create 3D structures are available in the *Sentaurus™ Structure Editor User Guide*.

Initial Structure Generation

The following examples show how to use geometric etching and deposition steps to generate simple initial structures in Sentaurus Topography 3D.

Simple Trench

This example shows how to create a simple silicon trench:

```
# Define a silicon unit cuboid as the initial bulk structure.  
define_structure material=Silicon point_min={0 0 0} \  
    point_max={0.24 0.05 0.33}  
  
# Define a cuboid shape that is used to etch a trench out  
# of the initial structure.  
define_shape type=cube name=trench point_min={0.06 0.0 0.15} \  
    point_max={0.18 0.05 0.33}  
  
# Use the shape to etch a trench.  
etch shape=trench  
  
# Save the final structure to file.  
save file="Structures/trench.tdr"
```

Fill

This example illustrates the use of the `fill` command when generating an initial structure:

```
# Define a silicon unit cube as the initial bulk structure.  
define_structure material=Silicon point_min={0 0 0} \  
    point_max={0.35 0.05 0.07}  
  
# Fill the initial structure with aluminum with a thickness  
# of 0.08 micrometers.  
fill material=Aluminum thickness=0.08  
  
# Fill again with Photoresist with a thickness of 0.18 micrometers.  
fill material=Photoresist thickness=0.18  
  
# Define a first cuboid shape that is used to etch a first trench  
# out of the previously generated structure.  
define_shape type=cube name=cuboid1 point_min={0.07 0.0 0.07} \  
    point_max={0.14 0.05 0.33}  
  
# Define a second cuboid shape that is used to etch a second trench  
# out of the previously generated structure.  
define_shape type=cube name=cuboid2 point_min={0.21 0.0 0.07} \  
    point_max={0.28 0.05 0.33}  
  
# Etch the two cuboids.  
etch shape=cuboid1  
etch shape=cuboid2  
  
# Save the final structure to file.  
save file=Structures/etch_input.tdr
```

Mask or Patterning

This example illustrates the use of the `define_mask` and `pattern` commands:

```
# Define an initial substrate.  
define_structure material=Silicon point_min={0 0 0} point_max={1 1 1}  
  
# Define a mask  
# - the mask is loaded from the file 'mask.gds'.  
# - the Sentaurus Topography 3D internal name is 'mask_1'.  
# - the layer used from the file 'mask.gds' is called '1:0'.  
# - the domain cut from the layer '1:0' is the rectangle {0 0} {1 1}.  
define_mask name=mask_1 file=mask.gds layer=1:0 \  
    domain_min={0 0} domain_max={1 1}  
  
# Pattern using 'mask_1' and material Photoresist.  
pattern mask=mask_1 material=Photoresist thickness=0.1
```

Appendix A: Examples

Initial Structure Generation

```
# Save the resulting structure to TDR.  
save
```

Multi-Tapered 3D Shapes

The following example defines a multi-tapered 3D shape with tilting angles:

```
# Define an initial structure.  
define_structure material=Nitride point_min={0 0 0} point_max={1 1 3}  
  
# Define a mask based on 2D polygon coordinates.  
define_mask name=m polygon={-5 0.7 -5 0.3 5 0.3 5 0.7}  
  
# Define the vertical tapered mask by specifying tapering angles.  
define_shape name=s type=mask mask=m \  
    z_coordinates={3.0 2.5 2.0 1.5 1.0} taper_angles={-10 15 0 -5}  
  
# Etch the mask.  
etch shape=s  
  
# Save the final structure.  
save
```

The following example defines multi-tapered 3D shapes by a 2D mask and a series of sidewall profile coordinates:

```
# Define an initial structure.  
define_structure material=Nitride point_min={0 0 0} point_max={1 1 3}  
  
# Define a mask based on 2D polygon coordinates.  
define_mask name=m polygon={-5 0.7 -5 0.3 5 0.3 5 0.7}  
  
# Define the sidewalls of the mask with pairs of lateral offsets  
# and z-coordinates.  
define_shape name=s type=mask mask=m \  
    profile={ 0.000 3.0 \  
        -0.088 2.5 \  
        0.046 2.0 \  
        0.046 1.5 \  
        0.002 1.0 }  
  
# Deposit the Photoresist mask.  
deposit shape=s material=Photoresist  
  
# Save the final structure.  
save
```

Deposition

The following examples show the use of the deposition models in Sentaurus Topography 3D.

Atomistic Layer Deposition

This example illustrates the atomistic layer deposition (ALD) model:

```
# Define an ALD machine and set the deposited material, the sticking
# coefficient, the anisotropy, the conformality, the growth per cycle,
# the cycle duration, and the ion angular distribution exponent.
define_deposit_machine model=ald material=Tungsten \
    sticking=1e-3 anisotropy=0 conformality=10 \
    growth_per_cycle=0.0001 cycle_duration=1 exponent=1

# Create an initial structure with a hole by removing a tapered cuboid
# from a block of Nitride.
define_structure material=Nitride \
    point_min={-0.1 -0.4 -5.1} point_max={0.1 0.4 0}
define_shape type=cube name=trench \
    point_min={-0.1 -0.1 -5} point_max={0.1 0.1 0} scale_bottom_y=0.9
etch shape=trench
save

# Start the ALD process.
deposit spacing=0.02 cycles=500 engine=monte_carlo

# Save the final structure to a file.
save
```

Crystallographic Orientation–Dependent Deposition

This example illustrates the crystallographic orientation–dependent deposition model:

```
# Define a crystal deposition machine, set the deposition rates
# along the <100>, <110>, and <111> directions of the lattice,
# set the deposited material, and set the material where deposition
# will occur.
define_deposit_machine model=crystal material=Silicon \
    selective_materials=Silicon rate_100=0.3 rate_110=0.1 \
    rate_111=0.01

# Create the initial structure and save it.
define_structure material=Silicon point_min={0 0 0} \
    point_max={0.03 0.06 0.18} slice_angle=-90
define_shape type=cube name=c0 point_min={0.01 0.02 0.14} \
    point_max={0.02 0.04 0.18}
```

Appendix A: Examples

Deposition

```
define_shape type=cube name=c1 point_min={0 0 0.05} \
    point_max={0.03 0.02 0.18}
define_shape type=cube name=c2 point_min={0 0.04 0.05} \
    point_max={0.03 0.06 0.18}
define_shape type=cube name=c3 point_min={0 0 0.05} \
    point_max={0.03 0.02 0.15}
define_shape type=cube name=c4 point_min={0 0.04 0.05} \
    point_max={0.03 0.06 0.15}
define_shape type=cube name=c5 point_min={0 0. 0.15} \
    point_max={0.01 0.06 0.2}
define_shape type=cube name=c6 point_min={0.02 0. 0.15} \
    point_max={0.03 0.06 0.2}

etch shape=c0
etch shape=c1
etch shape=c2

deposit shape=c3 material=Oxide merge=true
deposit shape=c4 material=Oxide merge=true
deposit shape=c5 material=Nitride
deposit shape=c6 material=Nitride

save

# Start the silicon deposition process and set the crystallographic
# orientation of the deposited region.
deposit spacing={0.002 0.002 0.002} time=0.25 } \
    flat_orientation={1 1 0 vertical_orientation={0 0 1}

# Save the final structure to a file.
save
```

Electrodeposition

This example illustrates the electrodeposition model:

```
# Define an electrodeposition machine and set its physical parameters.
define_deposit_machine model=electrodeposition material=Copper \
    overpotential=-0.21 bulk_distance=0.05 temperature=300 \
    depo_bulk_concentration=2.4e-4 exchange_current_density=1 \
    exchange_current_density_inh=0.039 \
    exchange_current_density_acc=2.5 inh_bulk_concentration=5e-8 \
    inh_diffusivity=5e-7 inh_adsorption_rate=6e4 \
    inh_displacement_rate=0 acc_bulk_concentration=0.64e-7 \
    acc_adsorption_rate=6e2 depo_diffusivity=4e-6 acc_diffusivity=1e-5

# Create an initial structure with a hole by removing a cuboid
# from a block of silicon.
define_structure material=Silicon point_min={-0.2 0} point_max={0.2 2}
define_shape name=hole type=rectangle point_min={-0.1 1.5} \
    point_max={0.1 2}
```

Appendix A: Examples

Deposition

```
etch shape=hole

# Start the copper deposition process and create a plot every
# 0.1 minutes.
deposit time=1.5 spacing=0.005 plot_interval=0.1

# Save the final structure to a file.
save
```

Electroplating Deposition

This example illustrates the electroplating deposition model:

```
# Define an electroplating deposition machine and set the
# deposited material, the rate, and the initial vertical
# change of the accelerator concentration.
define_deposit_machine model=electroplating material=Copper \
    rate=0.1 delta=5

# Create an initial structure with a hole by removing
# a cuboid from a block of silicon.
define_structure material=Silicon point_min={0 0 0} \
    point_max={1 1 1} region=bulk
define_shape type=cube name=hole point_min={0.3 0.3 0.5} \
    point_max={0.7 0.7 1.0}
etch shape=hole

# Start the copper deposition process and create a plot every 0.1 min.
deposit time=1 spacing={0.03 0.03 0.03} plot_interval=0.1

# Save the final structure to a file.
save
```

High-Density Plasma Deposition

This example illustrates the high-density plasma deposition model:

```
# Define a deposition machine that uses the hdp model
# and set the anisotropy, the ion angular distribution exponent,
# the deposited material, the rate, the redeposition
# coefficient, the sputtering coefficients,
# the sputter rate, and the sticking coefficient.
define_deposit_machine model=hdp material=Oxide rate=2.0 \
    anisotropy=0.7 exponent=100 redeposition=0.1 sputter_rate=0.95 \
    s1=5.5 s2=-6 sticking=0.1

# Load a structure from a file.
define_structure file=Structures/trench.tdr

# Start the oxide deposition process.
```

Appendix A: Examples

Deposition

```
deposit spacing={0.015 0.015 0.015} time=0.1  
# Save the final structure to a file.  
save
```

High-Density Plasma 2 Deposition

This example illustrates the high-density plasma 2 deposition model:

```
# Define a deposition machine that uses the hdp2 model  
# and set the anisotropy, the ion angular distribution exponent,  
# the deposited material, the rate, the redeposition coefficient,  
# the sputtering coefficients, the sputter rate,  
# the sticking coefficient, the sputtering distribution type,  
# the sputtering distribution exponent, and the reflection coefficient.  
define_deposit_machine model=hdp2 material=Oxide rate=2.0 \  
    anisotropy=0.7 exponent=100 redeposition=0.1 sputter_rate=0.95 \  
    s1=5.5 s2=-6 sticking=0.1 sputter_type="reflective" \  
    sputter_exponent=100 reflection=0.05  
  
# Load a structure from a file.  
define_structure file=Structures/trench.tdr  
  
# Start the oxide deposition process.  
deposit spacing={0.015 0.015 0.015} time=0.1  
  
# Save the final structure to a file.  
save
```

Low-Pressure Chemical Vapor Deposition

This example illustrates the low-pressure chemical vapor deposition model:

```
# Define a deposition machine that uses the lpcvd model  
# and set the deposited material, the rate,  
# and the sticking coefficient.  
define_deposit_machine model=lpcvd material=Oxide rate=1.0 \  
    sticking=0.35  
  
# Load a structure from a file.  
define_structure file=Structures/trench.tdr  
  
# Start the oxide deposition process.  
deposit spacing={0.015 0.015 0.015} time=0.2  
  
# Save the final structure to a file.  
save
```

Appendix A: Examples

Deposition

Physical Vapor Deposition

This example illustrates the physical vapor deposition model:

```
# Define a deposition machine that uses the pvd model
# and set the deposited material, the rate, and the ion
# angular distribution exponent.
define_deposit_machine material=Oxide model=pdf rate=1.0 exponent=1

# Load a structure from a file.
define_structure file=Structures/trench.tdr

# Start the oxide deposition process.
deposit spacing={0.015 0.015 0.015} time=0.15

# Save the final structure to a file.
save
```

Plasma-Enhanced Chemical Vapor Deposition

This example illustrates the plasma-enhanced chemical vapor deposition model:

```
# Define a deposition machine that uses the pecvd model
# and set the anisotropy, the ion angular distribution exponent,
# the deposited material, the rate, and the sticking coefficient.
define_deposit_machine model=pecvd material=Oxide rate=1.0 \
    anisotropy=0.6 exponent=30 sticking=0.05

# Load a structure from a file.
define_structure file=Structures/trench.tdr

# Start the oxide deposition process.
deposit spacing={0.015 0.015 0.015} time=0.2

# Save the final structure to a file.
save
```

Simple Deposition

This example illustrates the use of the simple deposition model:

```
# Define a deposition machine that uses the simple deposition model
# and set the deposited material, the curvature, and the rate.
define_deposit_machine model=simple material=Oxide rate=1.0 \
    anisotropy=0.3 curvature=0.1

# Load a structure from a file.
define_structure file=Structures/trench.tdr
```

Appendix A: Examples

Deposition

```
# Start the deposition process.  
deposit spacing={0.015 0.015 0.015} time=0.1  
  
# Save the final structure to a file.  
save  
  
# Extract the intersection points of the final structure  
# with a line passing through the point (0.05 0.05 0.0)  
# and parallel to the z-axis.  
extract type=1d_cut axis=z point={0.05 0.05 0.0}
```

Spin-on-Glass Deposition

This example illustrates the spin-on-glass deposition model:

```
# Define a deposition machine that uses the spin_on model  
# and set the deposited material, the viscosity, the density,  
# the initial_thickness, the radial_distance, the surface_tension,  
# the angular_velocity, the evaporation_rate, and the angular_position.  
define_deposit_machine model=spin_on material=Oxide viscosity=0.015 \  
    density=1 initial_thickness=2 radial_distance=2e4 \  
    surface_tension=27 angular_velocity=4000 \  
    evaporation_rate=0 angular_position=0  
  
# Create the initial structure and save it.  
define_structure material=Silicon point_min={0 0 0} \  
    point_max={100 100 1}  
define_shape type=cube name=11 point_min={40 0 1} point_max={60 100 4}  
define_shape type=cube name=12 point_min={0 60 1} point_max={60 80 2.5}  
define_shape type=cube name=13 point_min={60 30 1} \  
    point_max={100 50 1.5}  
deposit shape=11 material=Aluminum  
deposit shape=12 material=Aluminum  
deposit shape=13 material=Aluminum  
  
save  
  
# Start the oxide deposition process.  
deposit spacing={10 10} time=0.01 cfl=0.025  
  
# Save the final structure to a file.  
save
```

Appendix A: Examples

Etching

Etching

The following examples show the use of the etching models in Sentaurus Topography 3D.

Crystallographic Orientation–Dependent Etching

This example illustrates the crystallographic orientation–dependent etching model:

```
# Define a crystal etch machine, set the etching rates along
# the <100>, <110>, and <111> directions of the lattice, and
# set the material to be etched.
define_etch_machine model=crystal rate_100=1 rate_110=1.2 \
    rate_111=0.1 etchable_material=Silicon

# Create the initial structure and save it.
define_structure material=Silicon point_min={0 0 0} \
    point_max={0.4 0.2 0.2} region=Silicon_region
fill thickness=0.05 material=Photoresist
define_shape type=cube point_min={0.1 0.05 0.2} \
    point_max={0.3 0.2 0.3} name=cuboid

etch shape=cuboid

save

# Set the crystallographic orientation of the region with
# the material to be etched.
set_orientation region=Silicon_region flat_orientation={1 1 0} \
    vertical_orientation={0 0 1}

# Start the etch simulation process.
etch spacing={0.004 0.004 0.004} time=0.2

# Save the final structure to a file.
save
```

Dry Etching

This example illustrates the dry etching model:

```
# Define a dry-etch machine.
# Define the material that is redeposited and set
# the sticking coefficient and the redeposition rate.
define_etch_machine model=dry deposit_material=Anyinsulator \
    sticking=0.035 rate=0.2

# Multimaterial etch.
# Define materials and set the machine-dependent properties:
# rates and sputtering coefficients.
```

Appendix A: Examples

Etching

```
add_material material=Oxide rate=2.0 s1=5.5 s2=-6
add_material material=Resist rate=0.1 s1=5.5 s2=-6
add_material material=Anyinsulator rate=0.1 s1=5.5 s2=-6

# Load a structure from a file.
define_structure file=Structures/dry_etch_input.tdr

# Start etch simulation process.
etch spacing={0.015 0.015 0.015} time=0.1

# Save the final structure to a file.
save
```

Wet Etching

This example illustrates the wet etching model:

```
# Define a wet etch machine and set the etchant diffusivity and
# the distance of the source plane from the topmost point of the
# structure under process.
define_etch_machine model=wet diffusivity=1e-2 source_distance=1

# Define materials to be etched and their rates.
add_material material=Silicon rate=1

# Create an initial structure with a hole by removing a cuboid
# from a block of silicon.
define_structure material=Silicon point_min={0 0 0} point_max={2 3 2}
fill material=Photoresist thickness=0.5
define_shape type=cube name=c point_min={1 1 2} point_max={2 2 2.5}
etch shape=c

# Start etch simulation process.
etch time=0.5 spacing=0.1

# Save the final structure to a file.
save
```

Simultaneous Etching and Deposition

This example illustrates the simultaneous etching and deposition (etchdepo) model:

```
# Define an etchdepo machine and set the ion angular distribution
# exponent. Define the material that is redeposited and set the
# sticking coefficient and the redeposition rate.
define_etch_machine model=etchdepo exponent=100 \
deposit_material=Anyinsulator sticking=0.035 rate=0.2

# Multimaterial etch.
# Define materials and set the machine-dependent properties:
```

Appendix A: Examples

Etching

```
# rates and sputtering coefficients.  
add_material material=Oxide rate=2.0 s1=5.5 s2=-6  
add_material material=Anyinsulator rate=0.1 s1=5.5 s2=-6  
  
# Load a structure from a file.  
define_structure file=Structures/dry_etch_input.tdr  
  
# Start etch simulation process.  
etch spacing={0.01 0.01 0.01} time=0.1  
  
# Save the final structure to a file.  
save
```

High-Density Plasma Etching

This example illustrates the high-density plasma etch model:

```
# Define a high-density plasma etch machine and set  
# its ion angular distribution exponent.  
define_etch_machine model=hdp exponent=15  
  
# Multimaterial etch.  
# Define materials and set the machine-dependent properties:  
# rates, anisotropy, and sputtering coefficients.  
add_material material=Aluminum rate=1.13 anisotropy=0.04 s1=5.5 s2=-6  
add_material material=Photoresist rate=0.663 anisotropy=0.95 s1=5.5 \  
s2=-6  
  
# Load a structure from a file.  
define_structure file=Structures/etch_input.tdr  
  
# Start etch simulation process.  
etch spacing={0.015 0.015 0.015} time=0.1  
  
# Save the final structure to a file.  
save
```

High-Density Plasma 2 Etching

This example illustrates the high-density plasma 2 etch model:

```
# Define a high-density plasma 2 etch machine and  
# set its ion angular distribution exponent.  
define_etch_machine model=hdp2 exponent=100  
  
# Multimaterial etch.  
# Define materials and set for each of them the machine-dependent  
# properties: rates, anisotropy, sputtering coefficients,  
# sticking coefficient, and sputter rate.  
add_material material=Aluminum rate=1.13 anisotropy=0.04 s1=5.5 s2=-6 \  
s3=-6
```

Appendix A: Examples

Etching

```
sticking=0.5 sputter_rate=1.0
add_material material=Photoresist rate=0.663 anisotropy=0.95 s1=5.5 \
s2=-6 sticking=0.0 sputter_rate=0.0

# Load a structure from a file.
define_structure file=Structures/etch_input.tdr

# Start etch simulation process.
etch spacing={0.015 0.015 0.015} time=0.1

# Save the final structure to a file.
save
```

Ion-Enhanced Etching

This example illustrates the ion-enhanced etching model:

```
# Define an ion-enhanced etch machine and set
# its ion angular distribution exponent.
define_etch_machine model=ion_enhanced exponent=10

# Multimaterial etch.
# Define materials and set the machine-dependent properties:
# rates, anisotropy, sputtering coefficients, and sticking coefficient.
add_material material=Aluminum rate=0.7 anisotropy=0.5 sticking=0.5 \
s1=5.5 s2=-6
add_material material=Photoresist rate=0.5 anisotropy=0.5 sticking=0.0 \
s1=5.5 s2=-6

# Load a structure from a file.
define_structure file=Structures/etch_input.tdr

# Start etch simulation process.
etch spacing={0.015 0.015 0.015} time=0.1

# Save the final structure to a file.
save
```

Ion-Milling

This example illustrates the ion-milling model:

```
# Define an ion-mill machine.
define_etch_machine model=ionmill

# Multimaterial etch.
# Define materials and set the machine-dependent properties:
# rates, anisotropy, and sputtering coefficients.
add_material material=Aluminum rate=0.505 anisotropy=1.0 s1=5.5 s2=-6
add_material material=Photoresist rate=0.18 anisotropy=1.0 s1=5.5 s2=-6
```

Appendix A: Examples

Etching

```
add_material material=Tantalum rate=0.18 anisotropy=1.0 s1=5.5 s2=-6

# Load a structure from a file.
define_structure file=Structures/etch_input.tdr

# Start etch simulation process.
etch spacing={0.015 0.015 0.015} time=0.1

# Save the final structure to a file.
save
```

PMI Simple Etching

This example illustrates the PMI simple etching model:

```
# Define a PMI simple etching machine.
define_etch_machine model=pmi_simple_etch

# Multimaterial etch.
# Define materials and set the machine properties.
add_material material=Silicon rate=0.3 anisotropy=0.3
add_material material=Oxide rate=0.1 anisotropy=0.0

# Load a structure from a file.
define_structure file=Structures/etch_input.tdr

# Start etch simulation process.
etch spacing={0.005 0.005 0.005} time=0.1 plot_interval=0.03

# Save the final structure to a file.
save
```

The source code for the PMI model is available in the file:

```
 ${STROOT}/tcad/${STRELEASE}/lib/sptopo3d/examples/pmi_simple_etch/
 pmi_simple_etch.cc
```

Reactive Ion Etching

This example illustrates the reactive ion etch model:

```
# Define a reactive ion etch machine and set
# its ion angular distribution exponent.
define_etch_machine model=rie exponent=100

# Multimaterial etch.
# Define materials and set the machine-dependent properties:
# rates and anisotropy.
add_material material=Aluminum rate=0.7 anisotropy=1.0
add_material material=Photoresist rate=0.5 anisotropy=1.0
```

Appendix A: Examples

Etching

```
# Load a structure from a file.  
define_structure file=Structures/etch_input.tdr  
  
# Start etch simulation process.  
etch spacing={0.015 0.015 0.015} time=0.1  
  
# Save the final structure to a file.  
save
```

Reactive Ion Etching 2

This example illustrates the reactive ion etch 2 model:

```
# Define a reactive ion etch 2 machine and set  
# its ion angular distribution exponent.  
define_etch_machine model=rie2 exponent=100  
  
# Multimaterial etch.  
# Define materials and set the machine-dependent properties:  
# rates, anisotropy, and the sticking coefficient.  
add_material material=Aluminum rate=0.7 anisotropy=1.0 sticking=0.5  
add_material material=Photoresist rate=0.5 anisotropy=1.0 sticking=0.0  
  
# Load a structure from a file.  
define_structure file=Structures/etch_input.tdr  
  
# Start etch simulation process.  
etch spacing={0.015 0.015 0.015} time=0.1  
  
# Save the final structure to a file.  
save
```

This example creates a structure from the beginning and shows how to set the parameter reflection. Microtrenching at the bottom of the trench is formed:

```
# Define the initial bulk structure.  
define_structure material=Silicon point_min= {0 0 0} \  
    point_max= {0.1 0.02 0.01}  
  
# Create an oxide and a photoresist layer.  
fill material=Oxide thickness=0.15  
fill material=Photoresist thickness=0.02  
  
# Remove part of the photoresist.  
define_shape type=cube point_min= {0.025 0.0 0.16} \  
    point_max= {0.075 0.02 0.19} name=subtract  
etch shape=subtract  
  
# Save the initial structure.  
save
```

Appendix A: Examples

Tilt and Units

```
# Define the rie2 machine.
define_etch_machine model=rie2 exponent=100

# Set and define the material-dependent parameters.
# Ion reflection is only considered to happen in the resist.
# No neutrals are considered.
add_material material=Photoresist rate=0.0 anisotropy=0.0 sticking=0.0 \
    reflection=0.05
add_material material=Oxide rate=1.0 anisotropy=1.0 sticking=0.0
etch spacing= {0.005 0.005 0.005} time=0.05

# Save the simulation results, appending them
# in the previously generated TDR file.
save
```

Simple Etching

This example illustrates the simple etching model:

```
# Define an etch machine using a simple model.
define_etch_machine model=simple

# Multimaterial etch.
# Define materials and set the machine-dependent properties:
# rate, anisotropy, and curvature factor.
add_material material=Silicon rate=0.5 anisotropy=0.3 curvature=0.0
add_material material=Oxide rate=0.1 anisotropy=0.0 curvature=0.0

# Load a structure from a file.
define_structure file=Structures/etch_input.tdr

# Start etch simulation process.
etch spacing={0.015 0.015 0.015} time=0.1

# Save the final structure to a file.
save
```

Tilt and Units

This example shows how to tilt the wafer using the parameters `tilt` and `rotation`. At the same time, nondefault units are set:

```
# Define a deposition machine that uses a simple deposition model
# and set the deposited material, the anisotropy, the curvature,
# and the rate. Tilt and rotation are also set for the machine.
define_deposit_machine model=simple material=Oxide anisotropy=1.0 \
    curvature=0.0 rate=0.05<um/min> rotation=90 tilt=45
```

Appendix A: Examples

Simulations With 2D Structures

```
# Load a structure from a file.  
define_structure file=Structures/trench.tdr  
  
# Start the oxide deposition process.  
deposit spacing={10<nm> 10<nm> 10<nm>} time=60<s>  
  
# Save the final structure to a file.  
save
```

Simulations With 2D Structures

This example shows how to use Sentaurus Topography 3D to run simulations on two-dimensional structures:

```
# Define a 2D initial structure.  
define_structure point_min={0 0} point_max={1 1} material=Silicon  
  
# Fill works exactly as for a 3D structure.  
fill material=Photoresist thickness=0.1  
  
# Define a rectangle.  
define_shape type=rectangle name=rect point_min={0.25 0.5} \  
    point_max={0.75 1.5}  
  
# Etch a trench geometrically, exactly as for a 3D structure.  
etch shape=rect  
  
# Define a simple deposition machine, exactly as for a 3D structure.  
define_deposit_machine model=simple material=Oxide rate=1.0 \  
    anisotropy=0.7 curvature=0.0  
  
# Deposit. Note that the size of the 'spacing' parameter value  
# must match the dimension of the structure.  
deposit spacing={0.025 0.025} time=0.2  
  
# Save the 2D structure to TDR.  
save
```

Integration With Sentaurus Process

This example shows how to use the functionality of Sentaurus Topography 3D from within Sentaurus Process. This is a Sentaurus Process command file. Note the use of the `init` and `struct` commands instead of `define_structure` and `save`, respectively. The `topo` command of Sentaurus Process calls all the functionality related to Sentaurus Topography 3D:

```
# Initialize Sentaurus Process with a trench.  
init tdr=Structures/trench.tdr
```

Appendix A: Examples

Integration With Sentaurus Process

```
# Define a deposition machine that uses the simple model.  
# Note the 'topo' prefix.  
topo define_deposit_machine model=simple material=Oxide rate=2.0 \  
    anisotropy=0.7 curvature=0.0  
  
# Start the Oxide deposition process.  
# Note the 'topo' prefix.  
topo deposit spacing= {0.015 0.015} time=0.1  
  
# Save the structure.  
struct tdr=simple_deposition
```

B

EAD File Format

This appendix describes the energy angular distribution (EAD) file format.

Description of the EAD File Format

EADs can be stored in a tabular file format, defining the values of the EAD at discrete positions (E, θ), where E denotes the energy and θ is the polar angle.

EAD values are given in units of flux per energy and angle, that is, mol/m²/s/eV. A global conversion factor allows you to easily convert the values to the prescribed unit. In addition, you can specify the mathematical format of the distribution, for example, if the distribution includes an isotropy factor cosθ.

The file consists of the following:

- The *header section* contains meta information about the data. The first line must be the file format specifier, followed by the version number. In [Figure 38](#), line numbering is provided for demonstration purposes only and refers to the following:

Line 1: Format specifier (for example, ead_table) followed by version number

Line 2: List of monotonically increasing energy values

Line 3: List of monotonically increasing polar angle values

Line 4: Global scaling factor for all EAD values

Line 5: Mathematical form of the distribution

The lines of the header section can be given in arbitrary order and must contain, at least, the energy and angle values. In general, empty lines are ignored.

- The *value section* contains the EAD values.

Appendix B: EAD File Format

Mathematical Conventions

Figure 38 Format of the EAD file

EAD values arranged in a matrix of size:
 <number of energy values> x <number of angle values>

1	ead_table 1.0				
2	energies [eV]:	195	200	205	210
3	angles [deg]:	0	20	40	60
4	conversion_factor:	1e-18			
5	distribution_format:	standard			
6	5.54e-04	5.57e-05	3.24e-07	5.89e-10	0
7	3.67e-04	6.25e-05	1.56e-07	3.01e-10	0
8	3.29e-04	9.71e-05	1.03e-07	2.04e-10	0
9	3.36e-04	1.72e-05	7.93e-07	1.71e-10	0
10	3.94e-04	3.47e-05	6.97e-07	1.67e-10	0
11	6.21e-04	9.69e-05	8.34e-07	2.09e-10	0

Energy ↓ → Angle

Mathematical Conventions

The total flux Γ of the imported EAD is computed by integrating the EAD. Different mathematical conventions are possible as follows:

- distribution_format=standard:
$$\int_{E_{\min}}^{E_{\max}} dE \int_0^{2\pi} d\phi \int_0^{\pi/2} \sin\theta d\theta \text{ EAD}(E, \theta) = \Gamma$$

- distribution_format=cos_convention:

$$\int_{E_{\min}}^{E_{\max}} dE \int_0^{2\pi} d\phi \int_0^{\pi/2} \sin\theta d\theta \text{ EAD}(E, \theta) \cos\theta = \Gamma$$

The following example uses the standard distribution format. If you specify the parameter flux when defining the species distribution, the EAD is normalized to the specified flux:

$$\int_{E_{\min}}^{E_{\max}} dE \int_0^{2\pi} d\phi \int_0^{\pi/2} \sin\theta d\theta \text{ EAD}(E, \theta) = \text{flux}$$

Special Cases

If you specify only one energy value E , then the flux is computed as:

$$\int_0^{2\pi} d\phi \int_0^{\pi/2} \sin\theta d\theta \text{ EAD}(E, \theta) = \Gamma$$

If you specify only one angle value θ , then the flux is computed as:

$$\int_{E_{\min}}^{E_{\max}} dE \int_0^{2\pi} d\phi \text{ EAD}(E, \theta) = \Gamma$$

If you specify only one energy value E and only one angle value θ , then the flux is computed as: $2\pi \text{ EAD}(E, \theta) = \Gamma$

The same convention is used to save special particle Monte Carlo (PMC) species distributions, such as:

- Unidirectional distributions with only one angle value
- Energy-independent distributions (angular distributions), where the energy is stored as 0
- Species distributions that are saved with `energy_min=energy_max` (in which case, only one slice of the distribution, that is, an angular distribution with `energy E=energy_min`, is saved)

Sampling From the Distribution

The following methods are available to extract energy and angle samples from the given EAD:

- Rejection method
- Inverse cumulative distribution function (CDF) method

You can specify the sampling method using the parameter `sampling_method` of the `define_species_distribution` command (see [define_species_distribution on page 337](#)). For example:

```
sampling_method=inverse_cdf  
sampling_method=rejection
```

Glossary

ALD

Atomic layer deposition.

anisotropy

The ratio of the directional deposition or etch rate to the total deposition or etch rate, which is a combination of a directional component and an isotropic component.

CCP

Capacitively coupled plasma.

CDF

Cumulative distribution function.

chemical vapor deposition (CVD)

The growth of the material from a gaseous medium containing a mixture of reactants that chemically interact and convert to the required material.

curvature-dependent deposition/etch

The deposition rate along a curved surface is a function of the local curvature, which smooths the surface as it evolves.

conformal structure

If all the regions of a structure share the same vertices and faces along region boundaries that touch each other, the structure is *conformal*. If vertices or faces on shared region borders are not part of both regions, the structure is *nonconformal*. Sentaurus Topography 3D needs conformal structures as input. Nonconformal structures can be made conformal when read into Sentaurus Topography 3D by setting the parameter `conformalize=true` in the `define_structure` command.

CVD

Chemical vapor deposition.

dry etching

An etching process that uses plasma gas as the reactive source.

EAD

Energy angular distribution.

etching

The process that removes materials from the wafer surface.

HDP

High-density plasma.

high-density plasma (HDP) deposition

A deposition process that uses high-density plasma sources to produce deposition precursors. Usually, this process results in simultaneous deposition and sputter etching of thin film on the wafer surface, due to highly energetic ions.

IAD

Ion angular distribution. It describes the angular flux distribution of ions in flux models, that is, the probability of an ion traveling at a certain angle.

ICP

Inductively coupled plasma.

IEAD

Ion energy and angular distribution. It describes the energy and angular flux distribution of ions in flux models, that is, the probability of an ion traveling at a certain energy and angle.

ion-milling

A synonym for ion-mill etch.

ion-mill etch

An etching process purely caused by physical sputtering of the surface by highly energetic ions. The sputter yield (the number of particles knocked off the surface per incoming ion) is a function of the angle between the surface normal and the direction of the incoming ion.

IUPAC

International Union of Pure and Applied Chemistry.

low-pressure chemical vapor deposition (LPCVD)

The deposition environment is at such a low pressure that particle-particle collision based on gas-vapor deposition is negligible compared to particle-surface collision. The particles travel between surfaces in a ballistic trajectory.

LPCVD

Low-pressure chemical vapor deposition.

MPI

Message passing interface.

NAD

Neutral angular distribution.

ODE

Ordinary differential equation.

PECVD

Plasma-enhanced chemical vapor deposition.

physical vapor deposition (PVD)

The condensation of material from its own vapors.

plasma-enhanced chemical vapor deposition (PECVD)

A chemical vapor deposition technique that uses a plasma chemical vapor discharge to enhance the deposition characteristics.

PMC

Particle Monte Carlo.

PVD

Physical vapor deposition.

reactive ion etch (RIE)

An etching process in which chemically reactive ions are the major source of the reaction that removes particles from the surface.

RF

Radio frequency.

RFM

Rate formula module.

RIE

Reactive ion etch.

Sentaurus Lithography

A microlithography process simulator.

shadowed element

When a surface element has no vertical line of sight to the source because another surface element blocks its view, the element is *shadowed*.

SLO

File format used by Sentaurus Lithography.

sticking coefficient

The statistical probability that an incoming precursor will stay on the surface and contribute to the deposition of thin film, contrary to bouncing back to the gas phase. It controls the conformality in a reemission process.

STP

Standard temperature and pressure. Since 1982, IUPAC has defined STP as a temperature of 273.15 K or 0°C and a pressure of 10^5 Pa.

TDR

File format used for TCAD Sentaurus tools.

VBE

Volume boundary extraction.