

# **Garand User Guide**

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**SYNOPSYS®**

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# About This Guide

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This guide describes the operation of the Synopsys® Garand device simulator for drift-diffusion simulations, the Garand MC device simulator for Monte Carlo simulations, and the Garand VE device simulator for variability analysis.

For additional information, see:

- The TCAD Sentaurus™ release notes, available on the Synopsys SolvNetPlus support site (see [Accessing SolvNetPlus on page 35](#))
- Documentation available on the SolvNetPlus support site

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## Conventions

The following conventions are used in Synopsys documentation.

Convention	Description
<b>Bold text</b>	Identifies a selectable icon, button, menu, or tab. It also indicates the name of a field or an option.
Courier font	Identifies text that is displayed on the screen or that the user must type. It identifies the names of files, directories, paths, parameters, keywords, and variables.
<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.
[]	Denotes optional parameters or options.
...	Indicates that parameters can be repeated as many times as necessary.
	Indicates a choice among exclusive options.

---

## Customer Support

Customer support is available through the Synopsys SolvNetPlus support site and by contacting the Synopsys support center.

## Accessing SolvNetPlus

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

To access the SolvNetPlus site:

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

## Contacting Synopsys Support

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

- Go to the Synopsys [Global Support Centers](#) site on [www.synopsys.com](http://www.synopsys.com). There you can find email addresses and telephone numbers for Synopsys support centers throughout the world.
  - Go to either the Synopsys SolvNetPlus site or the Synopsys Global Support Centers 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](mailto:support-tcad-us@synopsys.com) from within North America and South America
- [support-tcad-eu@synopsys.com](mailto:support-tcad-eu@synopsys.com) from within Europe
- [support-tcad-ap@synopsys.com](mailto:support-tcad-ap@synopsys.com) from within Asia Pacific (China, Taiwan, Singapore, Malaysia, India, Australia)
- [support-tcad-kr@synopsys.com](mailto:support-tcad-kr@synopsys.com) from Korea
- [support-tcad-jp@synopsys.com](mailto:support-tcad-jp@synopsys.com) from Japan

## **Part I: Garand: Drift-Diffusion Simulator**

---

This part of the *Garand User Guide* contains the following chapters:

- [Chapter 1, Introduction to Garand](#)
- [Chapter 2, Importing Device Structures](#)
- [Chapter 3, Simulation Setup](#)

# 1

## Introduction to Garand

---

*This chapter introduces the Garand device simulator.*

---

### Functionality of Garand and the Workflow

Garand is a three-dimensional, drift-diffusion, quantum-corrected statistical device simulator that self-consistently solves the carrier concentration and potential distribution coupled with current continuity throughout the simulation domain. The drift-diffusion model consists of the Poisson equation, which is solved to determine the electrostatic behavior within the device, while carrier transport is modeled by the current continuity equation for the majority carriers, where both the drift and diffusion components of the current are accounted for. Garand also uses the density gradient model of quantum corrections to account for quantum-mechanical confinement within the device structure.

Garand performs drift-diffusion simulations in simulation domains defined by a device structure generator. The initial simulation domain defines an idealized uniform device. Statistical variability sources are injected into the simulation domain by Garand itself. Variability sources can be included by specification in the simulator input file, which controls aspects of the drift-diffusion solution. Given a randomized simulation domain, drift-diffusion simulation determines the drain current given a set of contact bias values. You can perform simulations over a range of bias conditions or to determine the threshold voltage given a current criterion.

Statistical variability sources can be applied to construct a unique device, given the definition of a uniform device structure, by the random sampling of an appropriate statistical distribution. Although the process is randomized, it is tied to devices by their number in an ensemble to ensure the ensemble can be reproduced. Each source of variability is treated independently in this way such that, for example, the distribution of random discrete dopants within a particular device in an ensemble of 10000 has the same distribution regardless of whether other sources of variability are included, provided that the 3D doping profile has not changed (for example, due to line edge roughness).

Variability sources associated with random discrete dopants, line edge roughness, polycrystallinity of gate materials, and interface-trapped charges are activated and

configured from the simulator input file. Regions of the device affected by some variability sources can be controlled by users for an imported device structure.

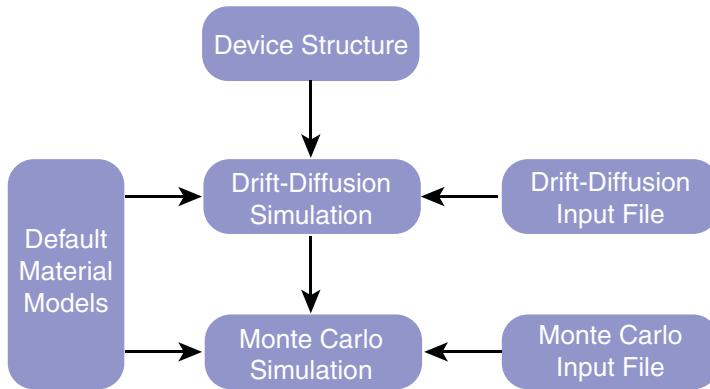
Carrier transport, as described by the current continuity equation, depends on carrier mobility. Garand includes standard mobility models to calculate the bulk mobility and to account for high-field effects. The mobility model parameters can be modified to calibrate I–V characteristics. These parameters are stored in the materials database and Garand provides an interface to override values in the materials database from within the simulator input file.

The extended capabilities of Garand allow for the simulation of arbitrary-shaped 3D MOSFET architectures. Garand offers direct import of TDR structure files, which must have a tensor-product mesh.

Garand is linked to an automated submission service, so that results pass automatically to a database for use with other elements of the workflow.

[Figure 1](#) shows how Garand fits into the workflow. Default materials in the simulation domain are defined jointly for both Garand and Garand MC, the Monte Carlo simulator, and are inputs to both. Nondefault materials can be specified using commands in the common input file for both simulators.

*Figure 1 Flow diagram showing relationship between Garand simulator and Garand MC simulator*



---

## Solution

The simulation domain is defined on a 3D rectilinear mesh, which provides an efficient discretization and solution scheme and is particularly important for efficient Monte Carlo simulations in which particle self-forces should be minimized. A steady-state solution is obtained by the self-consistent coupling of the electrostatic potential with majority and minority carrier concentrations. The solution is obtained iteratively by solving the nonlinear Poisson equation, obtaining a carrier concentration and field, followed by current continuity.

The nonlinear Poisson equation relates electrostatic potential to carrier density, where the carrier density itself is a function of the local potential and is described by a statistical distribution model. Current continuity then conserves the carrier flux given local mobility models.

## Unipolar

Garand is designed to simulate CMOS devices and assumes that the simulated transistor is unipolar. Concentrations for both majority and minority carriers are solved self-consistently with the potential throughout the simulation domain, but current continuity is solved only for the majority carriers.

## Nonlinear Poisson Equation: Carrier Statistics

The carrier concentration as a function of electrostatic potential for both majority and minority carriers is determined assuming the Boltzmann approximation to the Fermi–Dirac distribution function. Optionally, you can apply Fermi–Dirac statistics to determine the carrier concentration in materials and at doping concentrations where degenerate effects become important.

## Quantum Corrections

Quantum corrections can be included in drift-diffusion simulations through the solution of the density gradient equation. This is coupled with both the nonlinear Poisson and current continuity solutions and can be applied to both majority and minority carrier distributions. In this model, quantum corrections amend the carrier distribution in regions of high carrier-density variation. The changed carrier density then defines an effective quantum potential, used in carrier transport.

In addition, an alternative quantum-correction scheme based on the solution of the Schrödinger equation is available and is applied in a similar way to the density gradient approach. This provides a more rigorous quantum-mechanical correction but at the expense of increased computational effort.

## Current Continuity

Current continuity is solved only for the majority carriers and assumes a single total mobility model applied to the total carrier distribution. This treats the transport of subpopulations associated with the semiconductor material band model identically. The field in which carriers are driven is taken to be the effective quantum potential in the case of a quantum-corrected simulation. Otherwise, the electrostatic potential defines the electric field.

---

## Starting Garand From the Command Line

You can start Garand from the command line as follows:

```
garand -f <string> [<other_command-line_options>]
```

Command-line options control certain aspects of the simulation, allowing you to override specifications in the input file as required.

*Table 1      Command-line options for Garand*

Option	Description
-f <string>	Mandatory. Sets the name of the input file. Include the path if the file is not in the current working directory.
-c   --compatible <string>	Loads any available material files to align to a different tool or previous version (see <a href="#">Parameter Compatibility on page 191</a> ). It also can load any available parameter set for tabulated bands (see <a href="#">Full Band Model on page 274</a> ) by specifying: -c tabulated
-d <integer>	Sets the device number to simulate from within the statistical ensemble. This option is mandatory if you run statistical variability simulations of an ensemble of $n$ devices, where you must specify which device number, from 1 to $n$ , to simulate. Otherwise, it defaults to 1.
-dv <float>	Specifies the equivalent of the <code>bias delta=&lt;float&gt;</code> command.
-h   --help	Prints help message and exits.
--legacy	Uses the old convention for PMOS simulations, that is, the same as for NMOS with positive applied gate and drain biases, and a positive drain current output.
--max_threads <integer>	Sets the maximum number of parallel threads to use when running Garand on a multicore system (see <a href="#">Parallel Execution on page 41</a> ).
-nv <integer>	Specifies the equivalent of the <code>bias ivpoints=&lt;integer&gt;</code> command.
-stype <integer>	Specifies the equivalent of the <code>simulation sim_type=&lt;string&gt;</code> command.

## Chapter 1: Introduction to Garand

### Parallel Execution

Table 1 Command-line options for Garand (Continued)

Option	Description
--threads <integer>	Sets the number of parallel threads to use when running Garand on a multicore system (see <a href="#">Parallel Execution</a> ).
--user-materials	Specifies that Garand reads the default material parameters from the <code>device_materials.mat</code> file, which it writes, for the current device.
-vd <float>	Sets the drain voltage. This option is mandatory if the drain voltage is <i>not</i> specified in the input file with the <code>bias drain=&lt;float&gt;</code> command.
--verbose	Generates verbose screen output. This is useful to check the convergence of the solution.
-vg <float>	Sets the gate voltage. This option is mandatory if the gate voltage is <i>not</i> specified in the input file with the <code>bias gate=&lt;float&gt;</code> command.
-vsub <float>	Specifies the equivalent of the <code>bias substrate=&lt;float&gt;</code> command.

Garand can write a file (`device_materials.mat`) that contains a reduced list of default material parameters for *only* the materials that are actually in the device structure. This is activated with the command:

```
output user_materials = on
```

When starting Garand with the `--user-materials` option, Garand reads material parameters from this file rather than reading the parameter files for all known materials. This speeds up the initialization of materials at the start of the simulation.

---

## Parallel Execution

You can run Garand and Garand MC in parallel in multicore computing environments. You can specify the number of threads on the command line by using the `--threads` option. For example:

```
garand --threads 4
```

**Note:**

If you define multiple different values on the command line, then the simulator exits with an error.

Alternatively, you can specify the number of parallel threads to use in the input file by using the command:

```
simulation threads=4
```

**Note:**

As with other input file parameters, if multiple values are supplied, then the simulator uses the last value. Command-line specifications override any values set in the input file.

You can also use the `--max_threads` command-line option, which sets an upper limit for the number of threads to use, limiting values supplied in the input file or on the command line. As with the `--threads` option, supplying multiple different values causes the simulator to exit with an error.

The recommended approach for controlling the specification of these parameters is by using the options on the **Parallelization** tab in Sentaurus Workbench (see [Figure 2](#)), where the **Threads** and **Maximum Threads** fields correspond to the `--threads` and `--max_threads` options.

If you select **Auto-Detect**, then Sentaurus Workbench scans the processed input files to find the maximum number of threads requested. If you do not select **Auto-Detect**, then a value not less than 1 can be entered, with Sentaurus Workbench `@..@` notation accepted. For details, see the *Sentaurus™ Workbench User Guide*.

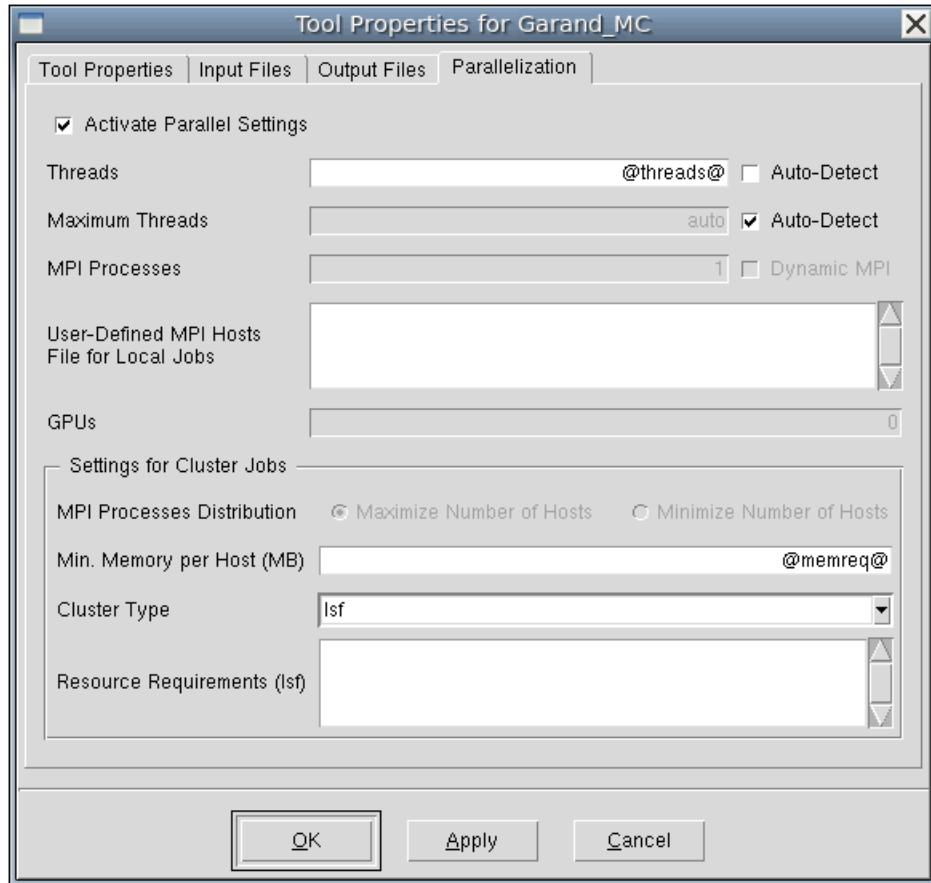
Where Garand is used to provide the initial guess for Garand MC (see [Monte Carlo Transfer Files on page 48](#)), serial execution is enforced for the drift-diffusion simulation, by default, to ensure reproducibility of the Garand MC simulation. Parallel execution can be used by setting the input file command:

```
SIMULATION enforce_serial_for_mct = off
```

## Chapter 1: Introduction to Garand

### Setting Up an Input File

Figure 2 Tool Properties dialog box for Garand MC showing Parallelization tab



---

## Setting Up an Input File

Garand input is based on a set of commands followed by assignment of parameters.

---

### Simulation Setup

The `simulation` command controls the behavior of Garand (see [simulation Command on page 884](#)). You must specify one parameter per line.

For example:

```
simulation sim_type = idvg
simulation n_or_p = p
simulation T = 275.5
simulation accept_unconverged = on
```

## Chapter 1: Introduction to Garand

### Setting Up an Input File

Garand operates in different modes depending on the setting of the `sim_type` parameter:

- If `sim_type=idvg`, then Garand calculates an  $I_d$ - $V_g$  curve (or single point).
- If `sim_type=idvd`, then Garand calculates an  $I_d$ - $V_d$  curve (or single point).
- If `sim_type=target`, then Garand searches for the gate voltage that produces a specified drain current.

These simulations are based on the bias conditions specified in the input file (see [Bias Conditions on page 98](#)).

Garand is a unipolar MOSFET simulator for NMOS and PMOS devices. You specify the type of device to be simulated using the `n_or_p` parameter, which controls whether the current continuity equation for electrons or holes is solved.

When running variability simulations of a statistical sample of  $n$  devices, each device is numbered from 1 to  $n$ . Running the same device number produces the same device structure each time (that is, the same random dopant distribution, line edge roughness, and so on). Changing the value of the `irand0` parameter introduces an offset in the seed number used by the random number generators and results in a different statistical ensemble that has the same device numbers.

The ambient temperature, in kelvin, is specified with the `T` parameter. The default is room temperature (300 K).

In Garand, the solution is usually very stable. Occasionally, particularly when using the local band-to-band tunneling model where the tunneling current dominates, the solution might oscillate between several very close values, leading to the assessment that the solution has not converged. On such occasions, Garand writes to the output file that the solution did not converge and the result is not passed to the database, thereby avoiding the accidental use of potentially erroneous results.

If you are confident that the solution will be close enough to be acceptable, then you can specify `accept_unconverged=on`. With this setting, Garand writes nonconverged results to the output file and passes the results to the database. Check such results carefully before using them.

If the solution for an I-V point does not converge, then Garand continues to simulate the other points in the I-V curve by default. If your preferred behavior is for the simulation to stop immediately if there is a nonconverged solution, then you can use the following command to cause the simulation to stop and fail without doing any further solutions:

```
simulation fail_on_unconverged=on
```

## Dimensional Unit

Many commands in the Garand input file require the specification of dimensions or positions within the device structure. Historically, the dimensional unit for all input and output was nanometer.

**Note:**

As the unit used in other Synopsys tools is usually micrometer, the output from Garand is in micrometer by default. However, to preserve backward compatibility for input files, input dimensions are still specified in nanometers by default.

Several commands control which units are used in input and output for the specification of distances, dimensions, and positions within the device structure.

To set both input and output units with one command, use:

```
structure units=<string>
```

To set only input units (overriding any units set with the `structure units=<string>` command), use:

```
structure input_units=<string>
```

To set only output units (overriding any units set with the `structure units=<string>` command), use:

```
output units=<string>
```

In all cases, <string> can be nm, um, mm, cm, or m.

**Note:**

Input units apply only when referencing dimensions and positions within the device structure, for example, bounding boxes, cutline positions, and line edge roughness (LER) planes. Model parameters, such as the root mean square and the correlation length of LER, and grain size for metal gate granularity, are still specified in nm.

---

## Device Structure

The `structure` command specifies certain aspects of the structure of the device being simulated (see [structure Command on page 899](#)).

If a metal gate is specified in the input file (`contact metal_gate`), then a workfunction for the gate material must be specified using the command:

```
contact work_function=<float>
```

## Chapter 1: Introduction to Garand

### Setting Up an Input File

For a polysilicon gate, the gate potential is determined by the doping concentration in the gate. You can also adjust the potential in a polysilicon gate, by adding the value specified to the potential set by the doping in the gate, with the following command:

```
contact poly_shift=<float>
```

See [contact Command on page 849](#).

---

## Mobility Models

You can specify up to five mobility models to use in a simulation, for each semiconductor material in the device, using the `material` command. See [Chapter 10 on page 313](#) for details.

For electron mobility in n-type MOSFETs, you specify:

```
material <material>.conduction.mobility.<model> <option>
```

For hole mobility in p-type MOSFETs, you specify:

```
material <material>.valence.mobility.<model> <option>
```

where `<model>` can be one of the following:

- `ball` selects the ballistic mobility model.
- `bulk` selects the low-field bulk mobility model (ionized impurity scattering).
- `elat` selects the lateral field-dependent mobility model (velocity saturation).
- `eprp` selects the perpendicular field-dependent mobility model (surface roughness scattering).
- `strain` selects the strain-dependent mobility model.

*Table 2 Options for mobility models*

Model	Option	Description
ball	none	Do not use a ballistic mobility model (default).
	shur	Use the Shur ballistic model.
bulk	constant	Use a constant value of mobility (default).
	arora	Use the Arora mobility model.
	masetti	Use the Masetti mobility model.
philips		Use the Philips unified mobility model.

## Chapter 1: Introduction to Garand

### Setting Up an Input File

Table 2 Options for mobility models (Continued)

Model	Option	Description
elat	none	Do not use a lateral field-dependent mobility model (default).
	caughey	Use the Caughey–Thomas velocity saturation model for the lateral field.
eprp	none	Do not use a perpendicular field-dependent mobility model (default).
	lombardi	Use the Lombardi mobility model for the perpendicular field.
thin_layer		Use the thin-layer mobility model.
	yamaguchi	Use the Yamaguchi mobility model for the perpendicular field.
strain	none	Do not use a strain-dependent mobility model (default).
	multivalley	Use the multivalley mobility model.
	sse	Use the simple strain enhancement model.

For example:

```
material Silicon.conduction.mobility.bulk masetti
material Silicon.conduction.mobility.eprp lombardi
material Silicon.conduction.mobility.elat caughey
```

Parameters for these mobility models are *material model* parameters. Therefore, you can use the `material` command to change the mobility model parameters for a particular material. For example:

```
material Silicon.conduction.masetti.mumin1 50.0
material Germanium.valence.caughey.vsat 9e6
```

---

## Capacitance Simulation

If you use the `simulation capacitance=<string>` command, then quasistatic capacitances,  $C_{ij} = \partial Q_i / \partial V_j$ , are calculated. Here,  $i$  and  $j$  each cover the following device contacts: gate (g), source (s), drain (d), and bulk (b). This involves performing extra solutions at each point of the I–V curve, which increases the simulation time.

By default, the full capacitance matrix is calculated, and each  $C_{ij}$  for the full I–V curve is written to a file. You can simulate a subset of the full capacitance matrix by specifying which responses of contacts to calculate. This is controlled by the `capacitance` parameter.

## Chapter 1: Introduction to Garand

### Setting Up an Input File

You can specify multiple comma-separated contacts in the capacitance specification to calculate the capacitance for multiple contacts. For example:

```
simulation capacitance=source  
simulation capacitance=gate,drain
```

The second command instructs Garand to calculate the capacitance for the gate and drain contacts only.

For each contact specified by the `capacitance` parameter, the bias on that contact changes by a small amount ( $\pm\Delta V_j$ ) and the charge in each of the contacts ( $\Delta Q_i$ ) is calculated. The capacitance  $C_{ij}$  is then calculated as:

$$C_{ij} = \frac{\Delta Q_i}{2\Delta V_j} \quad (1)$$

The  $\pm$  change in bias applied at each contact,  $\Delta V_j$ , can be changed by setting the parameters `cap_dv_drain`, `cap_dv_source`, `cap_dv_gate`, and `cap_dv_bulk` of the `simulation` command.

Two data columns are written to the output files: the first column is the gate or drain voltage (depending on the `sim_type` parameter) and the second column is the capacitance in farad (F). The capacitance output files are written to the results directory specified by the `output_directory=<string>` command and follow the same naming convention as the I-V data file (see [Output Files on page 166](#)). The capacitance matrix element,  $C_{ij}$ , that the file data represents is also included in the file name, for example, `device-idvg_vd0.05_Cgg_1.dat`. Capacitance results are also written to the output PLT file for plotting in Sentaurus Visual.

Capacitance data is also written to the database if it is activated for the simulation. This data is then available for compact model extraction in Mystic (see the *Mystic User Guide*).

---

## Monte Carlo Transfer Files

The Garand drift-diffusion simulator is used as a precursor to the Monte Carlo simulator, Garand MC. Using Garand to initialize Garand MC reduces the time for the Monte Carlo simulation to reach steady-state conditions by providing a solution of the simulation domain that captures the current transport and the electrostatics. Furthermore, it provides other simulation efficiency improvements by setting up a common mesh and simulation domain that are transferred using a Monte Carlo transfer (MCT) file, with the extension `.mct`.

An MCT file must be created for all bias points you want to simulate in Garand MC, and this file can be created only when either `sim_type=idvg` or `sim_type=idvd` is specified in the `simulation` command (see [Simulation Setup on page 43](#)). Garand creates one MCT file for each gate or drain bias point you sweep, so you can create an entire I-V curve of MCT files in one simulation run.

## Chapter 1: Introduction to Garand

### Setting Up an Input File

To specify that MCT files are created during an I–V curve simulation in Garand, use the following command:

```
output mc_transfer = on
```

By default, the `mc_transfer` parameter is switched off. Each MCT file is created in an MCT directory for each bias-dependent output directory. For more information about how the output of Garand is written, see [Monte Carlo Transfer File on page 174](#).

When MCT output is switched on, the following restrictions can affect Garand simulations:

- Monte Carlo simulations do not consider contact resistance, and contact resistance should be applied only in drift-diffusion simulations. Note that contact resistance does not directly affect carrier transport in the active region of a FET device and, therefore, it does not need to be captured in Monte Carlo simulations.
- Leakage models typically only apply in subthreshold conditions where a Monte Carlo FET simulation is not well suited. These models should be applied only in drift-diffusion simulations.
- The current continuity solution is required for MCT files for accurate Monte Carlo initialization. Only simulations examining long-channel conditions with `autoslice=on` or `remove_source_drain=on` can neglect the current continuity solutions. For further discussion, see [Long-Channel Simulation](#).
- Where drift-diffusion is run to produce an MCT file, serial execution is enforced to ensure reproducibility of results. Parallel execution can be used by setting:

```
SIMULATION enforce_serial_for_mct = off
```

---

## Long-Channel Simulation

There are certain circumstances where a full device simulation is not necessary, such as when evaluating the channel mobility in a Monte Carlo simulation assuming an infinite channel length, or when calibrating the density gradient solution under the gate of a long-channel device. In these cases, you can use the `remove_source_drain` parameter to remove the source/drain contacts and wells from the simulation domain leaving only the channel region. Removing source/drain contacts means that no bias voltage is applied (for mobility analysis in Monte Carlo simulations, a field can be specified; see [Long-Channel Simulations on page 230](#)).

### Note:

The lateral (the direction parallel to the source/drain plane) mesh specifications in the source/drain regions and even the channel can be relaxed significantly when using the `remove_source_drain` parameter. The only requirement is that the mesh is sufficiently fine to resolve the source/channel/drain regions.

The easiest way to do this is to use the `autoslice` parameter (see [Automatically Slicing a Structure on page 84](#)), as follows:

```
simulation autoslice=on
```

This command slices the center of the gate and creates a cross section that can be simulated using Garand MC with periodic boundary conditions.

A more flexible approach, which can be useful for Monte Carlo simulations, is to use the following command (see [Refining Automatic Slicing on page 231](#)):

```
structure remove_source_drain=on
```

However, this requires more user input. It is also advisable to ensure that quantum corrections are applied along the entire channel, which is achieved by specifying:

```
contact confined_boundary=on
```

For details, see [Long-Channel Simulations on page 230](#).

---

## TCAD Sentaurus Tutorial: Simulation Projects

The TCAD Sentaurus Tutorial provides various projects demonstrating the capabilities of TCAD to SPICE products.

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.

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

## Importing Device Structures

---

*This chapter discusses how to import device structures using TDR files.*

---

### Importing Structures From TDR Files

A 2D or 3D TDR structure file can be read in to Garand. To import a device structure, you must specify a TDR file to load with the command:

```
structure import filename='structure.tdr'
```

where `structure.tdr` is the name of the TDR file to be imported. This TDR file **must** be based on a 2D or 3D tensor-product mesh; otherwise, the command fails.

Device structures generated from process and topography simulation are based on a tetrahedral mesh in TDR format, while input structures for Garand (as well as Garand VE and Garand MC) must use a rectangular tensor-product mesh. An essential step in the TCAD to SPICE flow is the conversion of the process-simulated structure from a tetrahedral mesh to a tensor-product mesh.

You can use the tensor meshing scheme (with incorporated doping) of Sentaurus Mesh to convert the incoming finite-element mesh to a mesh suitable for simulation with Garand. To produce a file in TDR format that can be imported into Garand, call Sentaurus Mesh from the command line:

```
snmesh <file_name>.msh
```

**Note:**

Garand requires a 3D simulation mesh. Therefore, if a 2D TDR file is imported, then the 2D structure is extruded automatically in the z-direction by one mesh cell with a thickness of 1 nm. To simulate a structure with a different width, you must define a mesh in the z-direction. See [Specifying a Mesh on page 52](#).

For more information about converting a mesh for use by Garand, see the Sentaurus Mesh module of the TCAD Sentaurus Tutorial, Section 7.6 Tensor Mesh for Garand VE (see [TCAD Sentaurus Tutorial: Simulation Projects on page 50](#)).

## Chapter 2: Importing Device Structures

### Importing a Mesh

If you intend to use the mesh from the TDR file as the simulation mesh in Garand (see [Specifying a Mesh on page 52](#)), then you must control the mesh quality at this stage to ensure that all the important features of the structure are sufficiently resolved, but that the mesh is not so large that it will result in slow simulations in Garand. See the *Sentaurus™ Mesh User Guide* for details.

The materials in TDR structures must be valid materials in Garand. If materials are present that are not valid Garand materials with the recognized material name (see [Appendix A on page 842](#)), then an error is generated and a mapping must be provided in the input file to map unknown material names to known Garand materials (see [Changing Materials on page 76](#)).

---

## Importing a Mesh

Instead of specifying a mesh in the Garand input file, you can directly use the mesh in a TDR file. To do so, use the command:

```
mesh import [xmin=<float>] [xmax=<float>] \
            [ymin=<float>] [ymax=<float>] \
            [zmin=<float>] [zmax=<float>]
```

By specifying the optional parameters `xmin`, `xmax`, and so on, you can limit the region of the TDR file to be used for the simulation domain.

You can have a `mesh import` command as well as Garand `mesh` commands, described in [Specifying a Mesh](#), in the same input file. In that case, first the mesh is imported from the TDR file, and then additional `mesh` commands are applied. This allows imported meshes to be refined, for example, to better resolve statistical variation in geometry from line edge roughness (LER), or to be coarsened, for example, to create a quasi-2D structure by defining a single mesh space in the width direction to speed up simulations.

**Note:**

If you reflect a structure with an imported mesh, then the imported mesh is reflected automatically to cover the reflected part of the structure. This does not apply to any additional user-specified meshing.

---

## Specifying a Mesh

You can import the simulation mesh directly from a TDR file (see [Importing a Mesh](#)). You can also specify a simulation mesh in the Garand input file.

The simulation mesh must be set up to cover the region of the TDR structure that should be simulated in Garand. The mesh is rectilinear and the mesh nodes in the x-, y-, and z-coordinate directions are specified independently. The mesh definition is controlled by

## Chapter 2: Importing Device Structures

### Specifying a Mesh

specifying the minimum and maximum extents of a mesh region and either the number of mesh spaces into which that region should be divided or the mesh step size that should be used. Multiple `mesh` commands can be given for any particular direction. If mesh regions overlap, then the mesh spacing specified in the later command takes precedence.

#### **Caution:**

In the Garand input file, all dimensions are specified in nanometers by default. To use a different unit in the input file for dimensions and positions in the structure, see [Dimensional Unit on page 45](#).

The `mesh` command specifies how to generate the Garand mesh. You must specify the particular direction in which the mesh is applied, and the syntax is flexible:

```
mesh x start=<xmin> end=<xmax> (spaces=<integer> | step=<float>)
      [first=<float>] [last=<float>]
mesh y start=<ymin> end=<ymax> (spaces=<integer> | step=<float>)
      [first=<float>] [last=<float>]
mesh z start=<zmin> end=<zmax> (spaces=<integer> | step=<float>)
      [first=<float>] [last=<float>]
```

For each direction, you must specify the start point (`start`), the end point (`end`), and either the number of mesh spaces (`spaces`) that should be in that region or the step size (`step`). Optionally, you can also set a specific length of the first mesh space (`first`), or the last mesh space (`last`), or both in the region.

If you specify either `first` or `last`, then the lengths of the remaining mesh spaces in the region increase or decrease geometrically to fill the region with the number of specified mesh spaces.

#### **Note:**

The `first` or `last` parameter cannot be specified with `step` because they would be conflicting specifications.

If you specify both the `first` and `last` parameters for a region, then you must *not* specify `spaces`.

Garand automatically generates a mesh where the mesh spacing changes geometrically from `first` to `last`, with the number of mesh spaces calculated to fit the length of the region. It might not be possible to generate a mesh sequence that fits in the length of the region when using the exact values of `first` and `last` specified. The actual `first` and `last` spaces used are reduced to values that generate a mesh that will fit the region, with the specified values being a guaranteed maximum mesh spacing.

#### **Note:**

A good starting point is to fill the simulation domain with a uniform 1 nm mesh. Check that this covers the region of the device that you want to simulate in Garand, to ensure there will be at least a 1 nm mesh spacing everywhere. You can

## Chapter 2: Importing Device Structures

### Specifying a Mesh

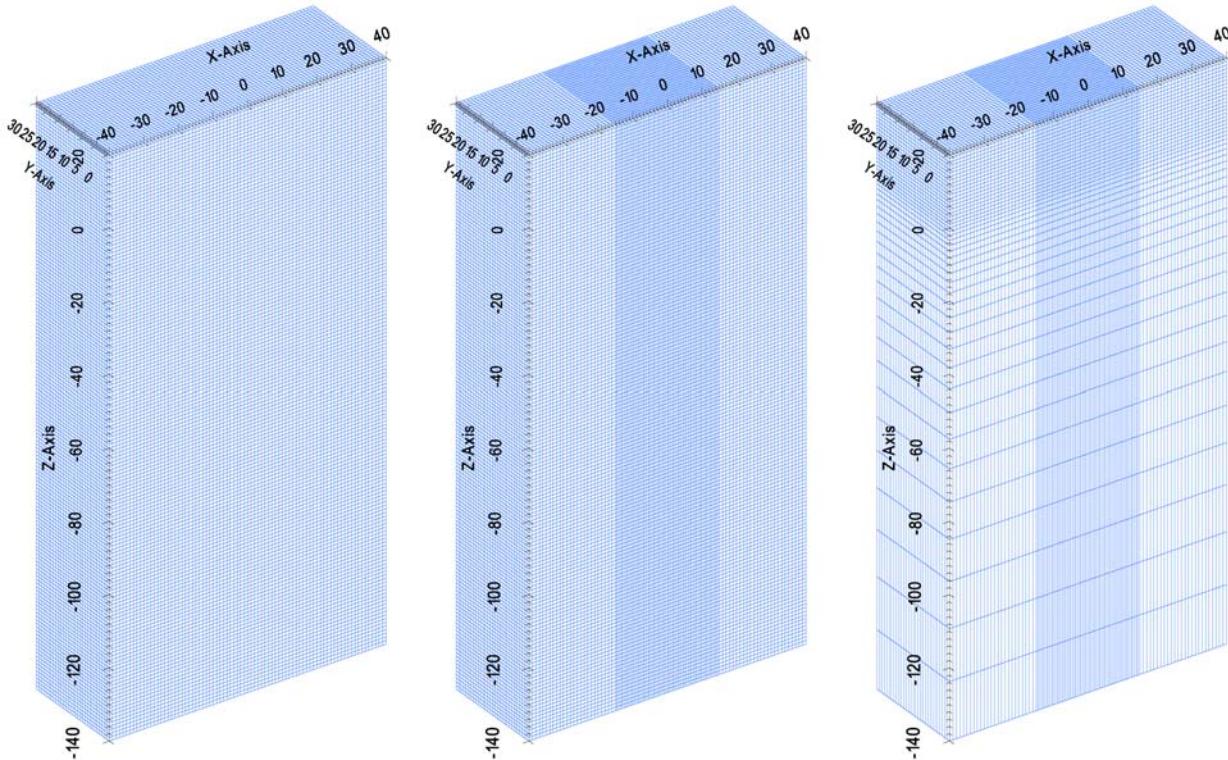
then make the mesh finer or coarser in specific regions to finely resolve certain features or to reduce the number of mesh nodes in regions, such as the substrate, where it is not necessary to have a small mesh spacing.

#### Example of Specifying a Mesh

These commands generate an 80 nm × 30 nm × 160 nm simulation domain with 1 nm mesh spacing in each direction, as shown in [Figure 3 \(left\)](#):

```
mesh x start=-40 end=40 spaces=80
mesh y start=0 end=30 spaces=30
mesh z start=-140 end=20 spaces=160
```

*Figure 3 Example of mesh generation steps*



The following command then overwrites the middle 30 nm in the x-direction with a 0.5 nm mesh spacing, for example, to resolve the MOSFET channel region, as shown in [Figure 3 \(middle\)](#):

```
mesh x start=-15 end=15 step=0.5
```

The next command replaces the mesh from z = -140 nm to 0 nm with 25 mesh spaces in such a way that the last mesh space (at z=0) will be 1 nm, as shown in [Figure 3 \(right\)](#):

```
mesh z start=-140 end=0 spaces=25 last=1
```

## Alternative Mesh Specification

An alternative method to specifying a mesh is simple but lacks some of the flexibility of the previously described method. In this alternative method, you specify a series of key mesh points (`pos`) with an associated mesh spacing (`dh`) in each of the x-, y-, and z-directions. For example:

```
mesh x pos=0.0 dh=1.0
```

The mesh spacing specified by the `dh` parameter is used as the mesh spacing on either side of the given position. Between key mesh points, the mesh spacing will change geometrically from the `dh` value at the first point to the `dh` value at the next point, in a similar way to specifying `first` and `last` in [Specifying a Mesh on page 52](#).

### Example

These commands demonstrate the alternative method, and [Figure 4 on page 56](#) shows the resultant mesh:

```
mesh x pos=0    dh=10      # P1
mesh x pos=25   dh=0.5     # P2
mesh x pos=30   dh=0.5     # P3
mesh x pos=50   dh=5       # P4
mesh x pos=70   dh=0.5     # P5
mesh x pos=75   dh=0.5     # P6
mesh x pos=100  dh=10      # P7
```

The mesh spacing starts at 10 nm at point P1. It then reduces geometrically to 0.5 nm at P2. As the spacing at P3 is also 0.5 nm, the spacing is uniform at 0.5 nm between P2 and P3. It then increases geometrically from 0.5 nm at P3 to 5 nm at P4. The sequence is then reversed through the remaining points to create a symmetric mesh.

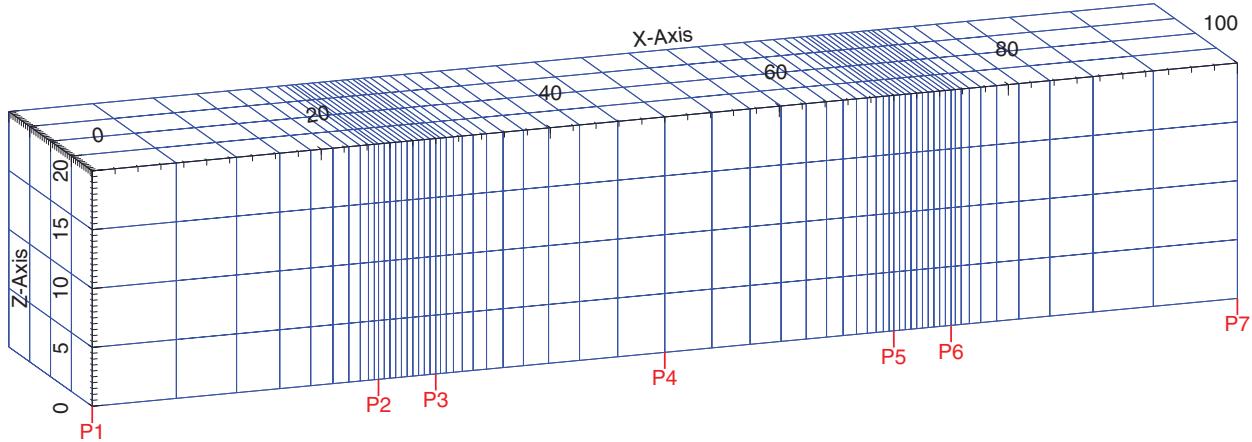
For comparison, the equivalent specification of the same mesh using the syntax described in [Specifying a Mesh on page 52](#) would be:

```
mesh x start=0  end=25   first=10  last=0.5    # P1 - P2
mesh x start=25  end=30   first=0.5 last=0.5    # P2 - P3
mesh x start=30  end=50   first=0.5 last=5      # P3 - P4
mesh x start=50  end=70   first=5   last=0.5    # P4 - P5
mesh x start=70  end=75   first=0.5 last=0.5    # P5 - P6
mesh x start=75  end=100  first=0.5 last=10     # P6 - P7
```

## Chapter 2: Importing Device Structures

### Specifying a Mesh

**Figure 4** Example of mesh generation using alternative method, showing key mesh points specified by each mesh command



---

## Automatically Specifying a Mesh

The `automesh` command allows the position of key mesh points described in [Alternative Mesh Specification on page 55](#) to be determined automatically, based on the location of transitions between materials. This is useful when simulating several structures where key device dimensions vary, so that a mesh line and given mesh spacing can always be specified at, for example, the start and the end of the gate when the gate length changes. This allows large design-of-experiments splits to be performed without having to manually adjust the mesh definition for each split.

The `automesh` commands are translated into `mesh` commands in the form described in [Alternative Mesh Specification](#), where a position and mesh spacing are specified, and they are then applied along with any `mesh` commands that are also in the input file.

You can see the autogenerated `mesh` commands in the `automesh.inp` file that can be written to the current working directory with the input file command:

```
output automesh=on
```

## Finding the Channel Region

To find the channel region, you must specify a material that surrounds the channel. This would typically be the gate oxide material.

In this example for a typical FinFET, the material specified is  $\text{HfO}_2$ . The channel is assumed to lie within the bounding box around the  $\text{HfO}_2$ , which is indicated in [Figure 5](#) by the magenta box in both graphics.

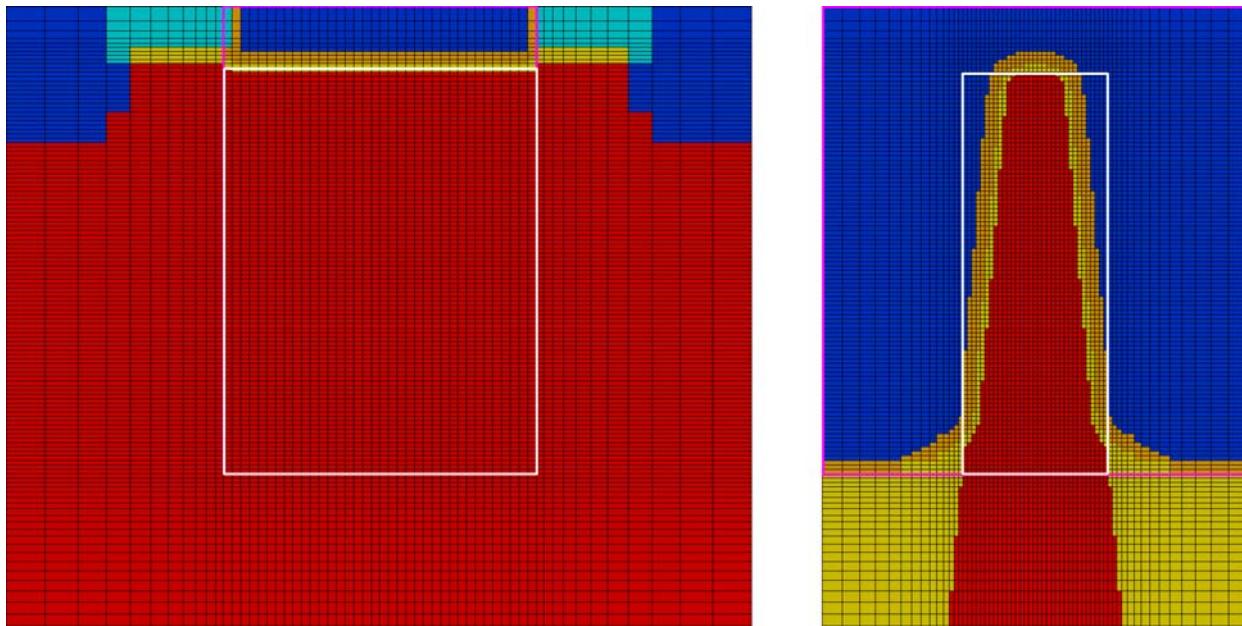
Garand then finds the tight bounding box that encompasses all of the semiconductor material that lies within the magenta box, which is indicated by the white box in both

## Chapter 2: Importing Device Structures

### Specifying a Mesh

graphics in [Figure 5](#). This white box defines the channel. In [Figure 5](#), a uniform mesh has been generated within the channel that is 1 nm in the y-direction (length) and 0.5 nm in both the x-direction (width) and the z-direction (height).

*Figure 5 Definition of the channel region in a FinFET*



Often, you need nonuniform meshing in the channel. Therefore, Garand allows you to specify a different mesh spacing at either side, in each direction. An option to specify a different mesh spacing in the middle of the channel is also available.

[Figure 6](#) illustrates 2 nm mesh spacing at the bottom of the fin, while retaining 0.5 nm at the top. A middle mesh spacing of 4 nm has been used in the y-direction (length) and 1.5 nm in the x-direction (width).

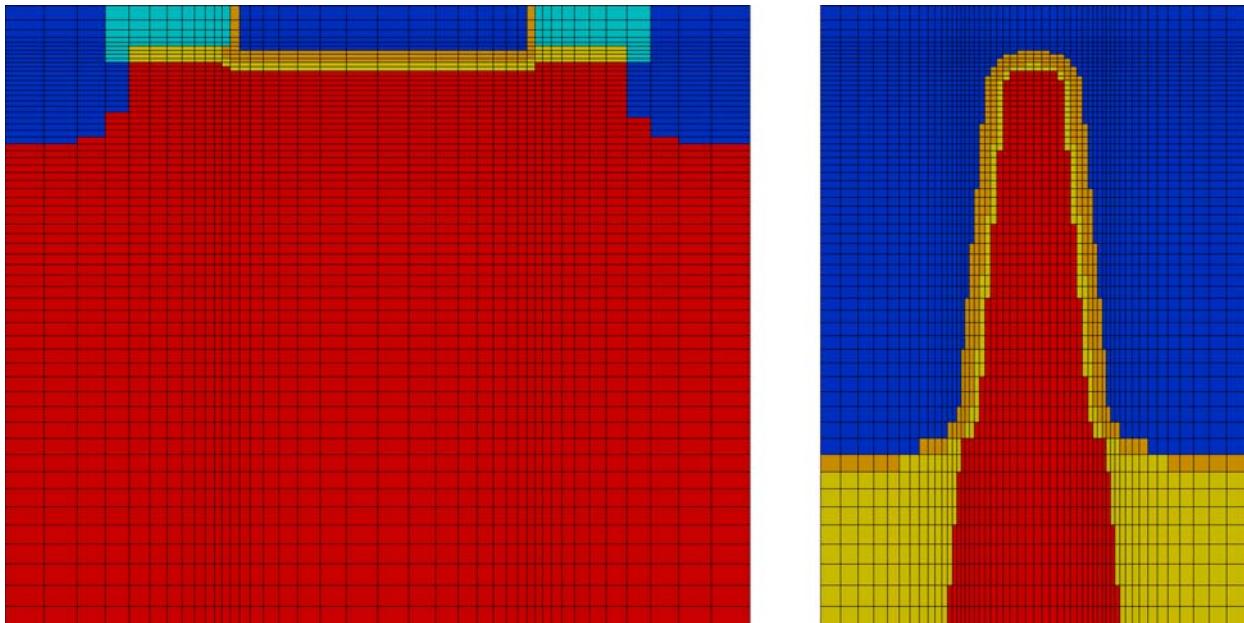
This can be specified in the input file with a command such as:

```
automesh channel mat=HfO2 dh_xstart=0.5 dh_xmid=1.5 dh_xend=0.5  
dh_ystart=1.0 dh_ymid=4.0 dh_yend=1.0  
dh_zstart=2.0 dh_zend=0.5
```

## Chapter 2: Importing Device Structures

### Specifying a Mesh

Figure 6 Nonuniform meshing of the channel region



## Finding Other Key Points

After the channel has been defined, it is useful to add other key points at significant transition points within a structure. To do this, you find the start and end points of contiguous blocks of material in each direction:

- The start is defined as a point of transition from a region where there is none of the specified material in the cross-sectional plane of the structure to a region where there is at least one element of that material in the cross-sectional plane.
- The end is defined as the reverse transition where there are no elements of the given material in the cross-sectional plane.

Each contiguous block is enumerated starting from the lowest coordinate point in each direction, so you can refer to the start of block 1 or the end of block 2, and so on.

As with the mesh specification described in [Alternative Mesh Specification on page 55](#), the `automesh` command requires a direction (x, y, or z) and a mesh spacing (`dh`) to be specified. The position (`pos`) of the mesh point to be added is determined from the material transition specified by the remaining `automesh` command parameters (`mat`, `block`, and `transition`).

In [Figure 7](#), you have added a key mesh point, with 0.5 nm mesh spacing, at the side of the silicon nitride (cyan material) closest to the source or drain.

## Chapter 2: Importing Device Structures

### Specifying a Mesh

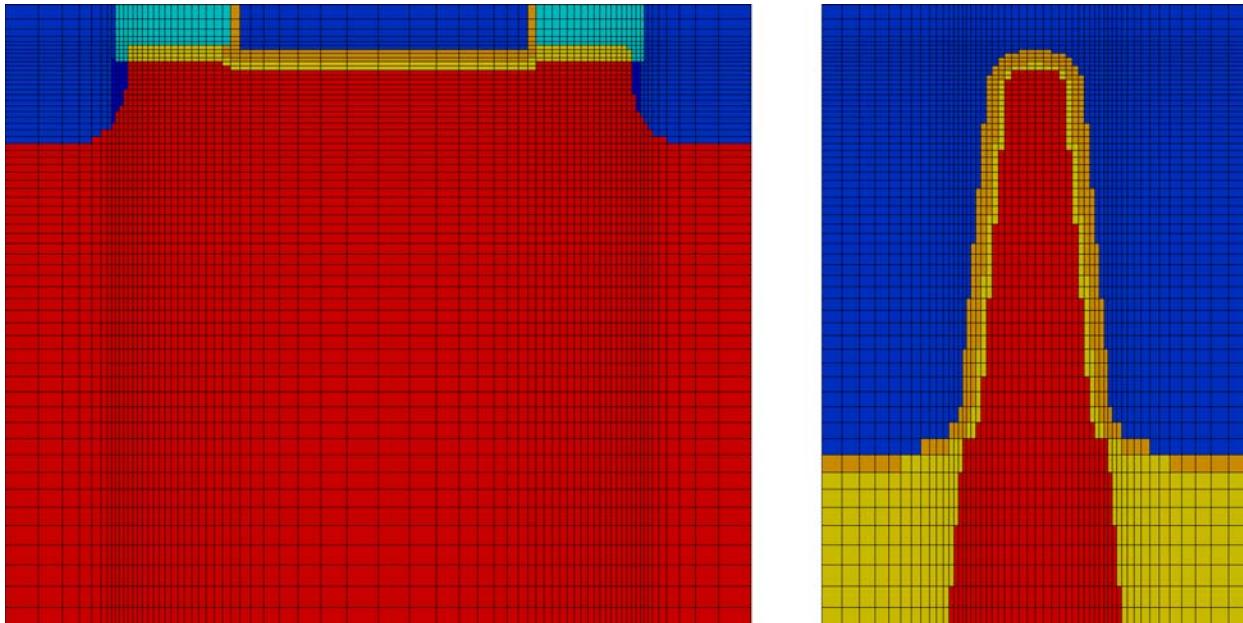
There are two blocks of silicon nitride: one in the source and one in the drain. Therefore, you can add a key point at the start of block 1 as follows:

```
automesh y dh=0.5 mat=Nitride block=1 transition=start
```

You can add a key point at the end of block 2 as follows:

```
automesh y dh=0.5 mat=Nitride block=2 transition=end
```

*Figure 7 Fine meshing at the ends of the spacers*



There is also a method to specify the mesh spacing between material transitions, for example, to coarsen the mesh. To do this, you must define the two material transitions that define the end points of the region, and then the specified mesh spacing will be applied at the midpoint between the two transitions.

If you want a 2 nm mesh spacing under the silicon nitride spacers, then you can specify them between the start of block 1 of nitride and the start of block 1 of HfO<sub>2</sub>. For example:

```
automesh y dh=2.0 mat=Nitride block=1 transition=start  
mat2=HfO2 block2=1 transition2=start
```

Likewise at the drain end:

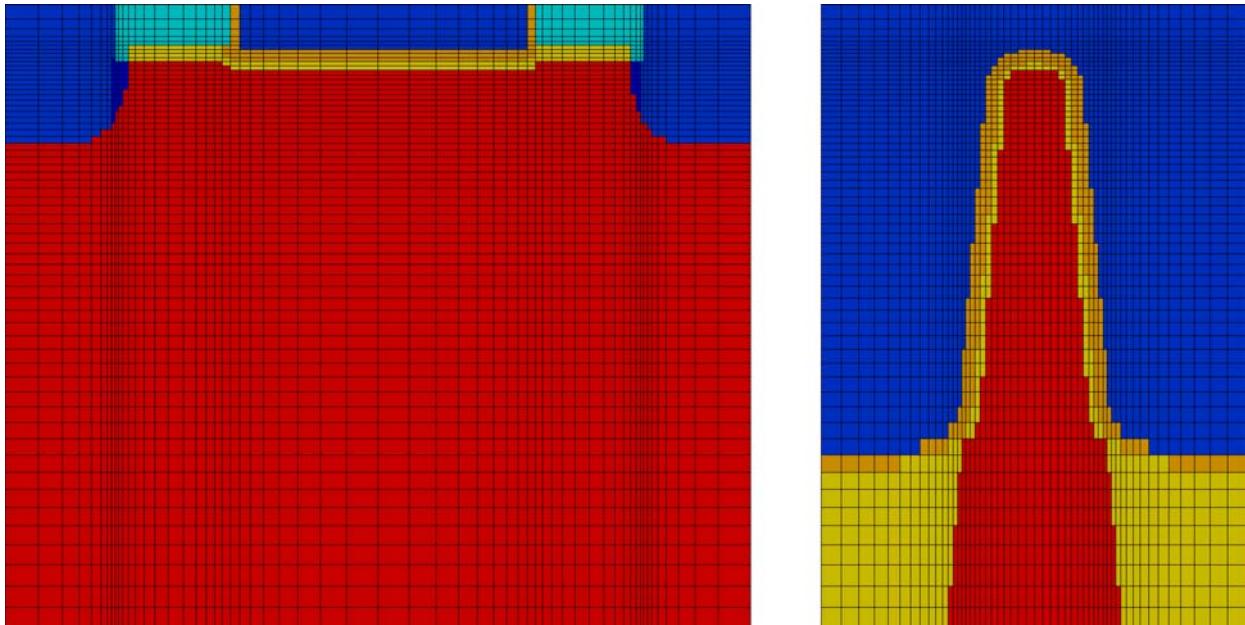
```
automesh y dh=2.0 mat=HfO2 block=1 transition=end  
mat2=Nitride block2=2 transition2=end
```

There are two blocks of nitride in the y-direction, but only one block of HfO<sub>2</sub>.

## Chapter 2: Importing Device Structures

### Reflecting Imported Device Structures

Figure 8 Coarser meshing in the middle of the spacer



An alternative way to automatically add a key mesh point at a position that is not exactly at a material transition point is to specify an offset from a given transition. This is performed by including the `offset` parameter in the `automesh` command. This offset value can be either positive or negative depending on which side of the transition point the mesh point should be added.

The following example adds a mesh point that is 10 nm *before* the first block of HfO<sub>2</sub>:

```
automesh y dh=2.0 mat=HfO2 block=1 transition=start offset=-10.0
```

The following example adds a mesh point that is 10 nm *after* the first block of HfO<sub>2</sub>:

```
automesh y dh=2.0 mat=HfO2 block=1 transition=end offset=10.0
```

---

## Reflecting Imported Device Structures

Sometimes, the structure imported into Garand is only half, or one quarter, of the entire device structure. Such a structure can be imported into Garand and then you can construct the entire device by reflecting the partial structure by using the following command:

```
structure reflect x+ | x- | y+ | y- | z+ | z- = on | off
```

You must specify one of the options for the direction in which to reflect the structure. For example, the `structure reflect x+=on` command reflects the structure in the positive x-direction around the maximum extent in that direction in the TDR file. Multiple reflections

## Chapter 2: Importing Device Structures

### Regions

can be specified. The following example reflects the structure in the positive x-direction and the negative y-direction:

```
structure reflect x+ = on
structure reflect y- = on
```

#### Note:

The simulation mesh specification, as described here, must cover the entire device structure after the reflections have been applied. For example, if the TDR file contains half of the device from  $y = 0$  nm to  $y = 25$  nm and a `structure reflect y-=on` command is applied to create the entire structure, then the Garand mesh must be defined from  $y = -25$  nm to  $y = 25$  nm.

---

## Regions

The structure in the TDR file to be imported consists of several different regions. Each region has one material associated with it. This region information is imported by Garand, and then specific regions can be targeted when modifying material properties or certain model parameters. When the Garand output TDR file is written, it will also contain the same regions. Therefore, region-specific visualization can be performed in Sentaurus Visual.

---

## Setting Region-Specific Material Parameters

Garand material parameters are described in [Chapter 8 on page 265](#). To change material parameters that apply to all regions of the structure containing that material, use the `material` command with the general form:

```
material <material>.<parameter> <value>
```

where:

- `<material>` is the name of a valid material (see [Appendix A on page 842](#)).
- `<parameter>` is a hierarchical material parameter.
- `<value>` is the new value to be assigned to the parameter.

The following commands change the material parameters universally and are applied to all regions that contain these materials:

```
material HfO2.permittivity    20.0
material Silicon.conduction.E 4.1
```

To change material parameters only in a specific region, you can modify the `material` command by replacing the material name with a specific region name. For example:

```
material <region>.<material_parameter> <value>
```

## Chapter 2: Importing Device Structures

### Regions

where <region> is the name of a region in which the material parameter should be modified.

#### Note:

Region-specific material parameter commands override any material parameter changes made to the general material.

The following commands change the permittivity to 4.5 in all occurrences of Oxide material, except in the region called Gate\_Oxide\_1, where it will change to 7.0:

```
material Oxide.permittivity      4.5
material Gate_Oxide_1.permittivity 7.0
```

By default, parameters are calculated based on the spatially varying mole fraction field. However, you can deactivate this by using the command:

```
simulation pos_dep = off
```

Here, the underlying material is SiliconGermanium. This will result in discrete materials being defined at each node by rounding the local mole fraction to the nearest 0.1. Therefore, regions will be defined based on a combination of region and material names. For example, for a mesh point contained within region Silicon\_1 with mole fraction 0.29, the resultant region will be called Silicon\_1\_Si70Ge30.

This offers an additional option when defining parameter values. So the following commands can be used to change the permittivity now:

```
material SiliconGermanium.permittivity    5.0
material Silicon_1.permittivity           6.0
material Silicon_1_Si70Ge30.permittivity 7.0
```

In this case, all SiliconGermanium materials in the simulation will have the permittivity 5.0, apart from those in the region called Silicon\_1, which will change to 6.0. Finally, the subregion called Silicon\_1\_Si70Ge30 will have permittivity 7.0.

---

## Adding User-Defined Regions

In general, regions in a TDR structure have been created by Sentaurus Process during process simulation. It is sometimes useful to have additional regions available in the structure when running drift-diffusion or Monte Carlo device simulations, to allow specific targeting of material parameters or the application of models to a part of the device structure.

You can add user-defined regions. By specifying a bounding box and a material name, all mesh elements that lie entirely within the bounding box and that currently contain the specified material are added to a newly created region, regardless of which region they currently belong to.

## Chapter 2: Importing Device Structures

### Doping Profiles

The command to add a new region is:

```
structure add_region name=<string> material=<string> \
    [new_material=<string>] \
    [xmin=<float>] [xmax=<float>] \
    [ymin=<float>] [ymax=<float>] \
    [zmin=<float>] [zmax=<float>]
```

For descriptions of the parameters of the structure `add_region` command, see [structure Command on page 899](#). All specified parameters must be on a single line in the input file.

Not all bounding box parameters need to be specified as they will default to the maximum extent of the device structure in the given direction. By default, the material of the new region will be the same as the material already in the elements that were added to the new region, that is, the material specified by the `material` parameter. You can choose a different material for the new region by including the optional `new_material` parameter. See [Appendix A on page 842](#) for a list of valid material names that can be used.

**Note:**

For a mesh element to be included in the new region, it must lie entirely within the specified bounding box. A tolerance of 0.1 nm is applied when determining this, to accommodate numeric rounding issues with the exact mesh positions.

---

## Doping Profiles

When you import an entire device structure from a TDR file, the doping within the device is included in that file and can be transferred to the Garand simulation mesh. Garand makes an assumption about which fields in the TDR file to import as donor and acceptor doping concentrations (see [Table 3](#)).

*Table 3 Default fields for different profiles*

Profile	Default fields
Net doping concentration ( $N_D - N_A$ )	DopingConcentration
Total doping concentration ( $N_D + N_A$ )	TotalConcentration
Total donor concentration ( $N_D$ )	DonorConcentration
Total acceptor concentration ( $N_A$ )	AcceptorConcentration
Donor dopant species	ArsenicActiveConcentration PhosphorusActiveConcentration

## Chapter 2: Importing Device Structures

### Doping Profiles

*Table 3 Default fields for different profiles (Continued)*

Profile	Default fields
Acceptor dopant species	BoronActiveConcentration IndiumActiveConcentration

To retrieve the total acceptor ( $N_A$ ) and donor ( $N_D$ ) concentrations, use the following procedure:

1. If DopingConcentration and TotalConcentration are present:

$$N_A = \frac{\text{TotalConcentration} - \text{DopingConcentration}}{2}$$

$$N_D = \frac{\text{TotalConcentration} + \text{DopingConcentration}}{2}$$

2. Otherwise, if total acceptor and donor concentration fields are present:

$$N_A = \text{AcceptorConcentration}$$

$$N_D = \text{DonorConcentration}$$

3. Otherwise, if dopant species fields are present:

$$N_A = \text{BoronActiveConcentration} + \text{IndiumActiveConcentration}$$

$$N_D = \text{ArsenicActiveConcentration} + \text{PhosphorusActiveConcentration}$$

4. Otherwise, if only DopingConcentration is present:

$$N_A = \begin{cases} 0 & \text{DopingConcentration} \geq 0 \\ |\text{DopingConcentration}| & \text{DopingConcentration} < 0 \end{cases}$$

$$N_D = \begin{cases} |\text{DopingConcentration}| & \text{DopingConcentration} > 0 \\ 0 & \text{DopingConcentration} \leq 0 \end{cases}$$

5. If none of these cases is met, then Garand stops with an error, as no suitable doping information has been found in the TDR file.

## Specifying Additional Doping Fields to Import

If you want additional dopant species fields in the TDR file to be included in the total donor and acceptor concentrations, then you can specify these additional fields in the Garand input file. To specify additional fields for donors and acceptors, use the following commands:

```
structure donor_fields = <string>
structure acceptor_fields = <string>
```

You must specify a comma-separated list of the names of all the fields to use, as labeled in the TDR file. For example, to explicitly reproduce the default behavior described in [Doping Profiles on page 63](#), the list of donor fields to import would be:

```
structure
donor_fields= ArsenicActiveConcentration,PhosphorusActiveConcentration
```

**Note:**

Some comments:

- If you specify a list of acceptor or donor fields, then these are the *only* doping fields imported. If you want the standard doping fields (such as BoronActiveConcentration) to also be used, then you must include them in the list.
- If you specify a list of acceptor\_fields in the input file, then you must also provide a list of donor\_fields, if there are any, and vice versa.

---

## Extra Doping From the DopingConcentration Field

By default, when importing doping from species fields, Garand compares the total acceptor or donor doping it has received with the net doping obtained from the DopingConcentration field. If the net doping shows a higher doping concentration, then Garand uses this instead. This ensures that any doping that has been added explicitly, in addition to the species doping, for example constant doping in a polysilicon gate, is included in the total acceptor or donor doping.

If a list of specific doping species fields is provided, however, then Garand assumes that these contain all the doping to be used, and the automatic comparison with net doping is deactivated.

To manually switch on this feature, include the following command in the input file:

```
structure extra_doping_from_net = on
```

Conversely, setting `extra_doping_from_net=off` deactivates this feature in all cases, so the feature will then not be used.

## User-Added Doping

Garand provides the option for you to add simple doping regions to the simulation structure or to replace doping that is already there. This is done with the `doping add` or `doping replace` command (see [doping Command on page 854](#)):

```
doping (add | replace) type=acceptor | donor \
    field=<string> peak=<float> material=<string> region=<string> \
    sigma-x=<float> sigma-y=<float> sigma-z=<float> \
    xmin=<float> xmax=<float> ymin=<float> ymax=<float> \
    zmin=<float> zmax=<float>
```

The `doping add` command adds the specified doping to any preexisting doping. The `doping replace` command removes any doping that is already in the region where doping should be added and replaces it with the new doping that is specified.

By providing a bounding box (`xmin`, `xmax`, and so on), the new doping can be restricted to a specific part of the simulation structure. Within this bounding box, a constant doping concentration, given by the `peak` parameter, will be added. Outside of the bounding box, the doping concentration will roll off with a Gaussian doping profile. The standard deviation of this Gaussian roll-off in each direction can be specified with the `sigma-x`, `sigma-y`, and `sigma-z` parameters.

This Gaussian roll-off is not applied if the `doping replace` command is used as this would replace the doping in the entire structure. In this case, the acceptor or donor doping will only be replaced within the bounding box with a constant doping concentration given by the `peak` parameter.

By specifying a `material` or `region`, the new doping (including any Gaussian roll-off) can be restricted so it is added only within the given material or region.

The new doping can be included in a specific doping field. This can be either a doping field that came from the imported TDR structure (for example, `BoronActiveConcentration`) or a new doping field specified with the `field` parameter. The doping will then be included in this doping field in the output TDR file. If random discrete dopants are being simulated, and `separate_species=on` (see [RDD From Separate Dopant Species Fields on page 101](#)), then the doping field containing the new doping can be included in the list of fields to be made discrete.

If no doping field is specified, then the doping is added to the `AddedAcceptorConcentration` field for acceptor doping or to the `AddedDonorConcentration` field for donor doping.

## Chapter 2: Importing Device Structures

### Importing Structures From Sentaurus Device TDR Files

---

## Importing Structures From Sentaurus Device TDR Files

In addition to using structures produced by Sentaurus Process as input structures, Garand can use TDR files produced as output from Sentaurus Device simulations. Such TDR files also must be remeshed, using Sentaurus Mesh, to have a tensor-product mesh.

The Sentaurus Device TDR file contains the same structural information (such as regions, materials, and contacts), and the doping concentrations will be obtained from the `DonorConcentration` and `AcceptorConcentration` fields.

One advantage of using a Sentaurus Device TDR file as input for Garand is that some of the parameters used for the Sentaurus Device simulation can be used directly in Garand without having to be calculated. This greatly assists the calibration of Garand to Sentaurus Device simulation results. Several options are available for parameter sets that can be used from the Sentaurus Device file, and these are described in the next sections.

---

## Importing Conduction Band and Valence Band Information

By importing the electron affinity and the effective band gap, the conduction and valence band edges can be set in a way that is consistent with Sentaurus Device, thereby including the effects of mole fraction, stress, and bandgap narrowing that have been applied in previous Sentaurus Device simulations.

To ensure that the carrier statistics used in the Garand simulation are consistent with the band profiles being imported, the electron and hole effective densities-of-states must also be imported. All these fields must be available in the Sentaurus Device TDR file.

Therefore, you must include the following data fields in the `Plot` section of the Sentaurus Device command file:

- `EffectiveBandGap`
- `ElectronAffinity`
- `eEffectiveStateDensity`
- `hEffectiveStateDensity`

If you use a Sentaurus Device TDR file as an input structure file for Garand and these data fields are in the file, then you can instruct Garand to import and use those fields using the command:

```
simulation import_bands = on
```

If all of the required data fields are not in the TDR file, then Garand generates an error and stops execution.

## Overriding the Imported Band Parameters

Occasionally, you might want to override the values of the imported band parameters; for example, if you have replaced one material with a different material and would like to use the default band parameters for that new material instead of the imported values. You can do this by providing a list of regions or materials in which the default band parameters for that region or material should be used, instead of the imported ones. This list is provided by using the following command:

```
simulation import_bands_override=<string>
```

For example:

```
simulation import_bands_override = PolySilicon
```

where PolySilicon is the material of the same name.

When the use of the imported band parameters has been overridden in a material or region, the values that should be used instead can be set in the usual way with a `material` command.

The following example sets the default value of the conduction band edge (that is, `ElectronAffinity`) and the valence band edge (that is, `ElectronAffinity + EffectiveBandGap`), respectively:

```
material PolySilicon.conduction.E 4.05  
material PolySilicon.valence.E 5.2
```

---

## Importing the Density-Gradient Calibration Parameter

By importing the density-gradient (DG) calibration parameter ( $\gamma$ ) used in Sentaurus Device, an equivalent parameter can be set in Garand so that it produces the same quantum correction as that obtained in Sentaurus Device.

This removes the need to calibrate the DG effective masses in Garand when comparing Sentaurus Device simulation results. Several other parameters are required to convert the  $\gamma$  parameter into the DG effective masses used in Garand; therefore, additional fields must be present in the Sentaurus Device TDR file.

You must include the following data fields in the `Plot` section of the Sentaurus Device command file:

- `eQDDGamma`
- `hQDDGamma`
- `eRelativeEffectiveMass`

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### Importing Structures From Sentaurus Device TDR Files

- hRelativeEffectiveMass
- StrainedDOSeMassFactor
- StrainedDOSHMassFactor

If you use a Sentaurus Device TDR file as an input structure file for Garand and these data fields are in the file, then you can instruct Garand to import and use those fields using the command:

```
simulation import_dg = on
```

If all of the required data fields are not present in the TDR file, then Garand generates an error and stops execution.

#### Note:

Some comments:

- Garand solves the DG equation everywhere in the device, which is particularly necessary when simulating random discrete dopants. If an eQPBox or hQPBox statement is specified in the Sentaurus Device command file, then Garand imports only the DG parameters inside the boxes defined by these statements. Outside of either box, the default DG effective masses, or those set for a material in the Garand input file, are used.
- To match the Sentaurus Device DG quantum correction completely in Garand, the same boundary conditions at oxide interfaces must be applied in both Sentaurus Device and Garand. See [Boundary Conditions at Oxide Interfaces on page 123](#) for how to apply Sentaurus Device boundary conditions in Garand, or vice versa.

## Overriding the Imported Density-Gradient Calibration Parameter

You can override the value of the imported DG calibration parameter ( $\gamma$ ) in one or more directions by values defined in the Garand input file. This is especially useful to avoid unwanted *tunneling* effects in the transport direction.

To override the  $\gamma$  parameter in the channel direction (automatically detected or specified), add the following command to the input file:

```
simulation import_dg_override_auto = on
```

Alternatively, specify the directions to override the  $\gamma$  parameter manually, by replacing `auto` with `x`, `y`, or `z`.

The following example overrides the imported  $\gamma$  parameter in the `x`- and `z`-directions by the default values, or those specified in the Garand input file:

```
simulation import_dg_override_x = on
simulation import_dg_override_z = on
```

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Importing Structures From Sentaurus Device TDR Files

### Limiting the Imported Density-Gradient Effective Mass

In Sentaurus Device, the DG equation is sometimes solved only within a specific bounding box set with `eQPBox` or `hQPBox`. If the DG  $\gamma$  parameter is imported into Garand, then this can cause a problem where the DG effective mass calculated for Garand at the boundary of this bounding box has a much higher value than that inside the bounding box or the default Garand parameter value used outside the bounding box. This can lead to instability in the Garand solution due to a large variation in the oxide boundary conditions over the short boundary transition region.

To prevent this, you can impose an upper limit on the DG effective mass obtained from the imported  $\gamma$  parameter, by using the command:

```
simulation import_dg_limit=<float>
```

The default value for this limit is 1.0. See [simulation Command on page 884](#).

---

### Importing the Dielectric Constant

The dielectric constant used in Sentaurus Device simulations can be imported from the TDR file. To do so, the prerequisites are:

- The element-based field `DielectricConstant` must be in the TDR file.
- Version P-2019.03 (or later) of Sentaurus Mesh must be used to convert the mesh in the TDR file to a tensor-product mesh.

To include the required field in the TDR file, add `DielectricConstant/Element` in the `Plot` section of the Sentaurus Device command file.

The `/Element` part is important. Without it, the `DielectricConstant` field would be written as a vertex-based field, rather than the element-based field required for Garand. It is this requirement for an element-based field that also necessitates the use of Version P-2019.03 of Sentaurus Mesh. In earlier versions, element-based fields were not remapped to the tensor-product mesh and, therefore, were removed from the converted TDR file.

To import the dielectric constant from the TDR file, specify the following command in the Garand input file:

```
simulation import_dielectric = on
```

If the element-based `DielectricConstant` field is found in the TDR file, then it is used to set the dielectric constant for each element of the simulation mesh; otherwise, Garand stops with an error.

## Chapter 2: Importing Device Structures

### Importing Structures From Sentaurus Device TDR Files

## Overriding the Imported Dielectric Constant

Occasionally, you might want to override the value of the imported dielectric constant, for example, to calibrate the permittivity of the gate dielectric. You can do this by providing a list of regions or materials in which the default dielectric constant for that region or material should be used, instead of the imported one. This list is provided by using the following command:

```
simulation import_dielectric_override = <string>
```

For example:

```
simulation import_dielectric_override = GATEox_1,HfO2
```

where `GATEox_1` is the region defining the gate oxide, and `HfO2` is the material of the same name.

When the use of the imported dielectric constant has been overridden in a material or region, the value that should be used instead can be set in the usual way with a `material` command. For example:

```
material GATEox_1.permittivity 5.0
material HfO2.permittivity 18.0
```

---

## Importing Mobility

By importing the mobility, the same mobility can be used in Garand as was used in Sentaurus Device, as long as the bias conditions for the Garand simulation match the bias conditions in the Sentaurus Device simulation that produced the TDR file. You must include the following data fields in the `Plot` section of the Sentaurus Device command file to ensure that the mobility is written to the TDR file:

- `eMobility`
- `hMobility`

If you use a Sentaurus Device TDR file as an input structure file for Garand and these data fields are in the file, then you can instruct Garand to import and use those fields using the command:

```
simulation import_mobility = on
```

This command imports the total mobility to use in the simulation. This does, however, introduce some restrictions to the Garand simulation if the mobility is imported:

- There is no freedom to modify or calibrate the mobility in Garand.
- If there is field-dependent mobility in the Sentaurus Device simulations, then you will need a Sentaurus Device TDR file with corresponding mobility for each I–V point at which Garand will be run.

## Chapter 2: Importing Device Structures

### Importing Structures From Garand TDR Files

The requirement to have a TDR file with the corresponding mobility for each bias point at which Garand will run is very restrictive. For this reason, there is the option to import the mobility from the TDR file and only to use it as the bulk low-field mobility in Garand. This bulk mobility should be valid at all applied biases, and high-field mobility effects should then be included with the relevant `eprp` and `elat` mobility models in Garand.

To import the mobility as only bulk mobility, use the command:

```
simulation import_bulk_mobility = on
```

The advantages are:

- The effects of stress, for example, on mobility should be accounted for in the bulk mobility in Sentaurus Device and, therefore, will be transferred into Garand.
- High-field mobility models can be applied in Garand and calibrated to match the I-V curves.
- Only one Sentaurus Device TDR file is required as the bulk mobility does not depend on the applied bias.

The disadvantage is that a Sentaurus Device simulation must be run with only a bulk mobility model activated, so that a valid mobility is imported.

---

## Importing Structures From Garand TDR Files

In addition to importing structures from Sentaurus Device TDR files (see [Importing Structures From Sentaurus Device TDR Files on page 67](#)), Garand can reimport structures from its own output TDR files. The Garand output TDR file is less general than that produced by Sentaurus Device, so there are some limitations on what can be imported from Garand TDR files, in particular, with regard to contacts.

To read a Garand TDR file as an input structure file, the standard command for specifying a structure file is used:

```
structure import filename=<string>
```

where `<string>` is the name of the Garand output TDR file, including the path if it is not in the current working directory.

In general, when running a Garand simulation that has read a structure from a Sentaurus Process or Sentaurus Device TDR file (after conversion to a tensor-product mesh), any data field that has been imported is written to the output TDR file and, therefore, is available to reimport when running a simulation that reimports that Garand output TDR file. In summary:

- The Garand simulation mesh is written to the output TDR file and becomes the default mesh when reimporting. This includes any bounding limits imposed on the original structure and any remeshing that was performed in the original Garand input file.

## Chapter 2: Importing Device Structures

### Importing Structures From Garand TDR Files

- Materials and regions from the Garand simulation are written to the output TDR file and, therefore, are read when reimplementing. This includes any material remapping and user-defined regions that were created in the original Garand simulation.
- The fields `AcceptorConcentration`, `DonorConcentration`, and `DopingConcentration` are always written to the output TDR file and, therefore, are read when reimplementing.
- Any imported dopant species field is written to the output TDR file and, therefore, is read when reimplementing.
- If an alloy fraction was read from `xMoleFraction`, then the `xMoleFraction` field is written to the output TDR file and, therefore, can be read when reimplementing.
- Unless their output has been deactivated explicitly, the fields `EffectiveBandGap`, `ElectronAffinity`, `eEffectiveStateDensity`, and `hEffectiveStateDensity` are always written to the output TDR file and, therefore, are read when reimplementing if `import_bands=on` (see [Importing Conduction Band and Valence Band Information on page 67](#)).
- `DielectricConstant` is always written to the output TDR file and, therefore, is read when reimplementing if `import_dielectric=on` (see [Importing the Dielectric Constant on page 70](#)).
- The majority carrier mobility (`eMobility` or `hMobility`) is always written to the output TDR file and, therefore, is read when reimplementing if `import_mobility=on` or `import_bulk_mobility=on` (see [Importing Mobility on page 71](#)).
- If `import_dg=on` was specified in the original Garand simulation, then the Sentaurus Device parameters that are imported with that setting are written to the Garand TDR file. They can be read when reimplementing.
- In the original Garand simulation, if a stress tensor was imported or defined in the Garand input file, and strain dependence was switched on in the input file, then the stress tensor is written to the TDR file and is available when reimplementing.
- Contacts are written as contact fields to the output TDR file and can be reimplemented using the `contact import=<string>` command.

---

## Importing the Solution From Garand TDR Files

The primary advantage for Garand rereading its own output TDR files is that it can import additionally the solution state from that file and use it as the initial conditions for a new simulation. By starting in an initial state that should be close to the final solution, this will reduce the simulation time and improve the solution stability.

## Chapter 2: Importing Device Structures

### Scaling the Output Current

Some examples where this approach might be beneficial are:

- When calibrating mobility parameters, import the solution from a previous set of mobility parameters when running with a new set of mobility parameters.
- When running statistical variability simulations, import the solution from a *uniform* simulation without variability.

To import the solution state from a Garand TDR file, use the command:

```
simulation import_solution=on
```

This allows the following fields to be imported from the TDR file:

- ElectrostaticPotential
- eDensity
- hDensity
- eQuasiFermiPotential or hQuasiFermiPotential

Data in these fields is used to initialize the electrostatic potential, the electron density, the hole density, and the majority-carrier quasi-Fermi potential in the structure.

To fully benefit from this feature, you need to import a Garand TDR file that was run at the initial bias conditions of the simulation you will be running. To ensure that the new simulation is run at the bias conditions specified in the input file, the contact boundary conditions are initialized according to those bias specifications, rather than the values obtained from the imported fields.

#### Note:

When using this feature, ensure that the Garand TDR file to be imported was obtained from a simulation that converged to a stable final solution.

In theory, you could import the solution from a Sentaurus Device TDR file, but this is not supported and is not guaranteed to work correctly.

---

## Scaling the Output Current

Garand outputs the current flowing through the structure being simulated in ampere.

If the simulation structure is *not* the entire structure (for example half of a FinFET), then you can scale the output current to give the total current for the entire structure by using the areafactor=<float> parameter.

The following example specifies that the area of the entire device is two times that of the simulated structure:

```
structure areafactor = 2.0
```

## Chapter 2: Importing Device Structures

### Specifying the Channel Direction

Therefore, the outputted current is multiplied by a scaling factor of 2.

---

## Specifying the Channel Direction

For certain operations and models, Garand must identify the channel direction (x, y, or z), that is, the direction in which current flows through the channel. Garand attempts to determine this automatically as being the direction in which the distance between the midpoints of the source and drain contacts is the greatest.

For most device architectures, this results in the correct assumption for the channel direction. However, for some novel architectures, this might produce an incorrect direction. In this case, or in general to ensure that Garand uses the correct direction, the channel direction can be specified in the input file by using the command:

```
structure channel_dir = x | y | z
```

---

## Specifying the Gate Length

In Garand, the gate length of the transistor is needed for the Shur mobility model (see [Shur Mobility Model on page 333](#)). Otherwise, the gate length is not used explicitly in Garand. However, the gate length of the simulated structure is written to the database, if database output is being used, because this information is needed within the database input files for Mystic (the Synopsys compact model extractor). For this reason, you must specify the gate length if Garand is saving results to the database.

If the gate length is not specified, then Garand attempts to estimate the gate length by calculating the distance between the maximum extents of the gate contact in the source-to-drain direction. For uniform device simulations, this is usually an accurate estimation. However, if there is gate edge roughness, then Garand calculates a different gate length for each statistical sample in the ensemble. This is sufficient for the Shur mobility model; however, this is not the correct value for compact model extraction as it should be the gate length of the nominal uniform device that is written to the database. With database output, you must explicitly specify the nominal gate length of the device by using the command:

```
structure gate_length=<float>
```

The gate length is given in nm, unless input units have been changed in the input file.

---

## Identifying Source and Drain Regions

For certain operations and models, Garand must identify the source and drain regions of the simulation structure. Garand searches for the contiguous region of majority-type doping that

## Chapter 2: Importing Device Structures

### Changing Materials

is in contact with the respective source and drain contacts, that is, the regions contained within the source or drain p-n junctions. In some structures with low-doped or undoped channels, however, there might not be a p-n junction between the source and drain contacts. In this case, Garand must decide how to differentiate between the source and drain regions.

By default, Garand assumes that the limit of the source or drain region is the midpoint of the simulation structure in the channel direction (see [Specifying the Channel Direction on page 75](#)). This is sufficient for most device architectures, but it might not work satisfactorily for some novel architectures.

An alternative method to determine the source and drain regions is available, based on finding the contiguous region of majority-type doping where that doping concentration is above a specified level. Therefore, even if there is no p-n junction between the source and drain contacts, as long as the doping concentration falls below the given level, the source and drain regions can be isolated from one another.

To specify the default behavior, using the middle of the structure in the channel direction as the division between the source and drain, use the following input file command:

```
structure limit_sd=middle
```

To specify the use of a doping limit to define the source and drain regions, use the following input file command:

```
structure limit_sd=doping
```

When using a doping concentration to define the limits of the source and drain regions, the doping concentration to use can be specified with the following input file command:

```
structure limit_sd_doping=<float>
```

The default doping concentration is  $10^{17} \text{ cm}^{-3}$ .

If the doping concentration used is too low, then it might not isolate the source and drain regions. If this happens, then Garand displays an error message with this information. In this case, increase the doping concentration by using the `structure limit_sd_doping=<float>` command.

---

## Changing Materials

If materials in the TDR file are not valid materials in Garand, then you must map these material names to the names of valid materials in Garand (see [Appendix A on page 842](#)) by using the command:

```
structure replace tdr_mat=<string> garand_mat=<string>
```

where `tdr_mat` is the name of a material used in the TDR file and `garand_mat` is the name of a valid material in Garand.

## Chapter 2: Importing Device Structures

### Specifying Contacts

This substitution is performed at the level of the TDR reader and applies to all regions in which the `tdr_mat` material is present.

---

## Changing Materials in Regions

After a structure has been imported into Garand, you can change the material of a region to a different Garand material using the command:

```
structure replace region=<string> garand_mat=<string>
```

where `region` is the name of a region and `garand_mat` is the name of a valid Garand material that will be associated with that region.

---

## Changing Materials Globally

You can also replace one material globally with a different material when importing a structure by using the command:

```
structure replace mat1=<string> mat2=<string>
```

where `mat1` is the material to be changed, and `mat2` is the material that will replace it.

**Note:**

This command changes all occurrences of `mat1` in the device structure.

However, you can no longer specify a bounding box for this material change, as it conflicts with the concept of one material per region. As the bounding box option was provided because there was no support for regions in Garand, it has now been superseded by the implementation of region support.

You can change materials on a region-by-region basis and, if you need to change the material within a given bounding box, then you can use the `add_region` option to create a new region within that bounding box where the material can be changed independently of existing regions (see [Adding User-Defined Regions on page 62](#)).

---

## Specifying Contacts

When importing a structure from a TDR file, you must instruct Garand where in the simulation domain to apply the different contacts. As the simulation mesh used in Garand is not necessarily the same as the mesh in the TDR file, a direct one-to-one mapping between contact nodes in the TDR file and nodes in the Garand mesh might not necessarily exist. This is further complicated by deformations in the Garand structure as a result of applied line edge roughness. Therefore, the specification of contacts in Garand is based on specifying a

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### Specifying Contacts

bounding box that encloses the contact, and the `filter` parameter that specifies which nodes within that bounding box are used as contact nodes.

To simplify the specification of contact locations, you can extract contact information from the TDR file as described here, and Garand attempts to generate the contact specification automatically, based on the position of contact nodes and the surrounding materials.

---

## Specifying Contact Locations

Contact locations are specified using the `contact` command (a backslash denotes a line continuation for the purposes of formatting in this manual only):

```
contact metal_gate filter=<string> [bias=<float>] [name=<string>] \
    [barrier=<float> | work_function=<float>] \
    [xmin=<xmin>] [xmax=<xmax>] \
    [ymin=<ymin>] [ymax=<ymax>] \
    [zmin=<zmin>] [zmax=<zmax>]
contact poly_gate filter=<string> [bias=<float>] [name=<string>] \
    [barrier=<float>] \
    [xmin=<xmin>] [xmax=<xmax>] \
    [ymin=<ymin>] [ymax=<ymax>] \
    [zmin=<zmin>] [zmax=<zmax>]
contact source filter=<string> [bias=<float>] [name=<string>] \
    [xmin=<xmin>] [xmax=<xmax>] \
    [ymin=<ymin>] [ymax=<ymax>] \
    [zmin=<zmin>] [zmax=<zmax>]
contact drain filter=<string> [bias=<float>] [name=<string>] \
    [xmin=<xmin>] [xmax=<xmax>] \
    [ymin=<ymin>] [ymax=<ymax>] \
    [zmin=<zmin>] [zmax=<zmax>]
contact substrate filter=<string> [bias=<float>] [name=<string>] \
    [xmin=<xmin>] [xmax=<xmax>] \
    [ymin=<ymin>] [ymax=<ymax>] \
    [zmin=<zmin>] [zmax=<zmax>]
contact ohmic filter=<string> [bias=<float>] [name=<string>] \
    [xmin=<xmin>] [xmax=<xmax>] \
    [ymin=<ymin>] [ymax=<ymax>] \
    [zmin=<zmin>] [zmax=<zmax>]
contact fixed_gate filter=<string> [bias=<float>] [name=<string>] \
    [barrier=<float> | work_function=<float>] \
    [xmin=<xmin>] [xmax=<xmax>] \
    [ymin=<ymin>] [ymax=<ymax>] \
    [zmin=<zmin>] [zmax=<zmax>]
```

Here, `xmin`, `xmax`, `ymin`, `ymax`, `zmin`, and `zmax` specify a bounding box within which the contact will be defined.

## Chapter 2: Importing Device Structures

### Specifying Contacts

#### Note:

It is not necessary to specify all the bounding box limits (`xmin`, `xmax`, and so on) as they will default to the maximum extent of the simulation domain in that direction.

## Naming Contacts

All contacts can be given a name by using the `name` parameter. This name is used as a label to identify the contact in data saved in the database. For example, the applied bias is labeled `V<name>`, where `<name>` is the name of the contact.

If the contact position has been imported from a field in the input TDR file (see [Importing Contact Locations on page 81](#)), then the contact is named, by default, after the TDR field from which it was imported. This can be overridden with the `name` parameter.

## Specifying a Filter

The `filter` parameter specifies a filter to determine which mesh nodes in the bounding box are assigned to the contact. Valid options are:

- `semiconductor`: Nodes that lie within and on the boundary of semiconductor regions
- `insulator`: Nodes that lie within and on the boundary of insulator regions
- `direct`: See [Importing Contact Locations on page 81](#)
- `metal`: Nodes that lie within and on the boundary of metal regions
- `polysilicon`: Nodes that lie within and on the boundary of polysilicon regions
- `void`: Nodes that lie within and on the boundary of void and Gas regions (void regions are also classed as insulators)
- `xmin`, `xmax`, `ymin`, `ymax`, `zmin`, and `zmax`: Nodes that are at the minimum or maximum extent of the simulation mesh in whichever direction is specified

#### Note:

You can set only one `filter` parameter per `contact` command. However, you can specify multiple `contact` commands for the same contact.

## Specifying the Bias

The bias applied at each contact is usually specified by a `bias` command. However, the `bias` parameter allows you to specify bias conditions when defining a contact with a `contact` command. The specification here follows the same rules as for the specification with a `bias` command (see [Bias Conditions on page 98](#)).

#### Note:

You can use only one method for specifying bias conditions on a contact, either using a `bias` command or specifying the `bias` parameter in the `contact` command. You still need to specify the other bias parameters, `ivpoints` and `delta`, in the `bias` command.

## Considerations

- If no nodes are found that match the criterion specified in the `contact` command for those contacts, then Garand terminates the simulation.

The only exception is if the `simulation solve=off` command is specified (see [Input File Options on page 164](#)), in which case, Garand sets up the device structure and outputs the TDR file without running a simulation. This is useful for debugging the mesh and contact specifications.
- Source, drain, substrate, and generic Ohmic contacts apply only to nodes that lie within and on the boundary of semiconductor regions. Therefore, if you choose `insulator`, `metal`, or `void` as the filter, then the contact applies only to nodes where those regions bound with semiconductor regions.
- Polysilicon gate contacts will apply only to nodes that lie within and on the boundary of polysilicon regions. Therefore, if you choose `insulator` or `void` as the filter, then the contact applies only to nodes where those regions bound with polysilicon regions.
- If you choose `metal` or `void` as the filter for source or drain contacts, then the region of metal or void material enclosed by the specified bounding box will be treated as a fixed-potential region. Therefore, the bounding box must include any regions to be treated as contact plugs. In addition, any other metal attached to the contact will be added to the fixed-potential region.
- If you include the input file command `contact void_fill=on`, then any void region attached to a contact with a `void` filter specification will be filled with a fixed-potential plug. This must be used only if the attached void regions are clearly isolated from any other contacts.
- In the context of a Garand simulation, an *Ohmic* contact is a generic contact to a semiconductor region that is not specifically the active drain, source, or substrate contact. The contact can have a fixed applied bias, specified by the `bias` parameter, which will not be ramped during an I–V sweep.
- In the context of a Garand simulation, a *fixed gate* refers to any gate contact in the structure that is not the active gate of the device being simulated and that will not have the applied bias ramped during an  $I_d$ – $V_g$  sweep. Each fixed gate can have its own workfunction and a fixed applied bias.

## Chapter 2: Importing Device Structures

### Specifying Contacts

- For fixed gate contacts, the workfunction and fixed bias can be specified on the contact definition statement. If omitted, then the default workfunction is that of the active metal gate, and the default bias is 0.0 V.
- For metal gate and fixed gate contacts, instead of specifying a workfunction, a barrier potential,  $\Phi_{MS}$ , can be specified. This barrier is the difference in the workfunction between the gate contact and the intrinsic reference semiconductor (see [Specifying the Metal Gate Workfunction on page 82](#)). Note that the `barrier` and `work_function` parameters cannot both be set in the same contact definition.
- If a barrier is specified for a poly gate, then the value given is applied as an offset to the Fermi potential in the polysilicon. A positive barrier will act to make the device threshold voltage more positive by the value given in volts (for both NMOS and PMOS). A negative barrier will act to make the threshold voltage more negative.
- If contacts specified as being metal gate or fixed gate contacts also make contact with regions of polysilicon, then any barrier applied to those contacts is also applied to the region of polysilicon in the same way as for a polysilicon gate.

---

## Importing Contact Locations

If the TDR file contains fields that define the locations of contacts, then these fields can be used to generate the bounding box and filter information automatically. To specify that the location of a contact should be taken from the TDR file, you must use the `import` parameter of the `contact` command to specify the name of the field that contains the contact location. In the following example, `source` is the name of the contact field in the TDR file:

```
contact source import='source'
```

Garand extracts the bounding box for the contact from the maximum and minimum extents of the contact field and attempts to set the filter based on the materials on which these contact points are bounding.

It is still possible to specify any of the bounding box values or filter as previously described, and these will override the values taken automatically from the TDR file.

When contact positions are imported from contact fields in the TDR file, the `direct` filter option instructs Garand to attempt a direct one-to-one mapping of the contact nodes in the TDR file to the structure on the simulation mesh. For example:

```
contact drain import='drain' filter=direct
```

If there is no remeshing of the structure in Garand, and no modification to the structure (for example, due to line edge roughness), then the one-to-one mapping should be very reliable.

To map contacts when the mesh or structure has been modified, each node in the simulation mesh is tested to see whether the nearest node in the imported TDR mesh is on a contact.

## Chapter 2: Importing Device Structures

### Specifying Contacts

If it is and the simulation mesh node is at the interface between two materials, then the simulation mesh node is included in the contact.

If the contact is defined on the boundary of a void–gas region, then it is a good idea to switch on the following option:

```
contact void_fill=on
```

In this case, Garand assumes that the entire void region attached to the contact should be part of the contact. This can help to catch nodes in the contact that might be missed when doing the direct mapping.

**Note:**

This works only if the void region is not also connected to another contact.

The contact fields must be present in any subsection of the entire structure that is being imported. As it is common to not import the entire structure, particularly omitting large substrates, it is possible that certain contacts, such as the substrate contact, might not be present in the imported subsection of the structure. In this case, you must specify the contact location manually. For substrate contacts, it is often sufficient to specify the side of the structure on which to apply the contact.

The following example applies the substrate contact to the side of the structure that has the minimum z-value:

```
contact substrate filter=zmin
```

If the structure should be reflected to create the drain from the source, or vice versa, then this reflection operation must occur *before* importing the structure into Garand, so as to produce two separate contacts that can be uniquely identified. If you apply the reflection in Garand, then both the source and drain contacts will be part of the same contact field and cannot be differentiated.

---

## Specifying the Metal Gate Workfunction

If a metal gate is specified for the structure, then a workfunction for the active metal gate **must** be specified by using the command:

```
contact work_function=<float>
```

The metal gate workfunction is given in eV.

You can also specify the workfunction in the contact definition command, as shown in [Specifying Contact Locations on page 78](#). This allows different parts of the active metal gate to be specified with different workfunctions by splitting the specification of the different parts of the gate into different contact definition commands.

## Chapter 2: Importing Device Structures

### Specifying Contacts

For fixed metal gates with a fixed potential, the workfunction is specified on the individual contact definition command, as shown in [Specifying Contact Locations](#). However, if the workfunction for a fixed metal gate is not specified, then it defaults to the value specified here for the active gate.

For both metal gate and fixed gate contacts, instead of specifying a workfunction, a barrier potential,  $\Phi_{MS}$ , can be specified. This barrier is the difference in the workfunction between the contact and the intrinsic reference semiconductor. The electrostatic potential on the contact,  $\phi_{con}$ , is then:

$$\phi_{con} = \phi_{ref} + V_{con} - \Phi_{MS} \quad (2)$$

where:

- $\phi_{ref}$  is the reference Fermi level (usually, 0.0 V).
- $V_{con}$  is the applied voltage on the contact.
- $\Phi_{MS}$  is the barrier potential as specified for the contact.

To specify the barrier potential, set the `barrier` parameter in the `contact` command that defines the contact (see [Specifying Contact Locations](#)).

---

## Setting Other Contact Options

When transferring from a finite element (FE) mesh to a tensor-product finite difference (FD) Garand mesh, it is likely that some nodes on the boundaries of semiconductor regions in the FD mesh will have very low doping as they lie within insulator regions in the FE mesh.

To avoid this problem at nodes within source/drain contacts, you can fill the contacts with a given level of doping using the command:

```
contact fill= <float> | max
```

where `<float>` is the doping concentration in  $\text{cm}^{-3}$  and `max` indicates the maximum value of doping.

The following example fills each node in the source and drain contacts with a doping concentration of  $1 \times 10^{20} \text{ cm}^{-3}$  of the majority-type doping for the contact (that is, n-type doping for an n-channel MOSFET or p-type doping for a p-channel MOSFET):

```
contact fill=1e20
```

The following example fills each node in the source and drain contacts with the maximum value of doping that already exists in that contact:

```
contact fill=max
```

## Chapter 2: Importing Device Structures

### Structural Modifications

For example, if the doping at nodes within the source contact ranges from  $6.7 \times 10^{17} \text{ cm}^{-3}$  to  $2.6 \times 10^{20} \text{ cm}^{-3}$ , then every node in the contact is filled with a doping concentration of  $2.6 \times 10^{20} \text{ cm}^{-3}$ .

Polysilicon gate contacts can be filled in a similar way by using the `polyfill` parameter:

```
contact polyfill=max  
contact polyfill=2e20
```

When contacts are defined on the boundary of metal or void (that is, gas–air) regions, Garand assumes that those regions form part of the contact. It uses a fill algorithm to find all the connected nodes in the metal–void regions that should form part of the contact. In certain cases, for void regions, this might not be the required behavior. Therefore, void regions are not automatically assumed to be part of the contact. To fill void regions attached to contacts, use the command:

```
contact void_fill=on
```

The boundary conditions for the density-gradient quantum corrections force a gradient in the carrier concentration at semiconductor–insulator interfaces.

As source/drain contacts sometimes lie at such interfaces, you can use the `confined_boundary` parameter to specify whether to apply the density-gradient boundary conditions within the contact:

```
contact confined_boundary= off | on
```

The default is `off`.

For the application of contact resistance, see [Contact Resistance on page 132](#).

---

## Structural Modifications

You can modify an imported structure using various parameters, which are primarily intended for use when running a calibration of quantum corrections or initial simulations for use in Garand MC.

Having large highly doped source and drain regions is not ideal when running Monte Carlo simulations because the majority of particles in the simulation are located in these highly doped regions and, therefore, do not contribute to the current through the channel, and their movements can lead to plasma oscillations.

---

## Automatically Slicing a Structure

When calibrating density-gradient quantum corrections against the more rigorous Poisson–Schrödinger solution, it is usually the inversion layer charge in the middle of the channel that

## Chapter 2: Importing Device Structures

### Structural Modifications

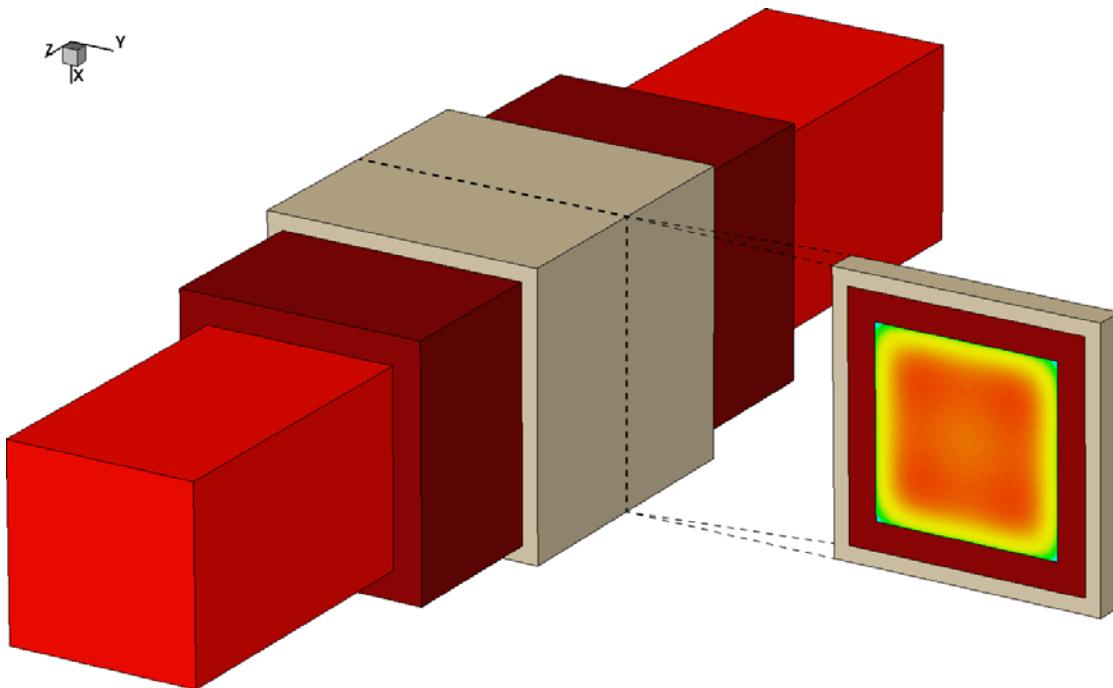
is of interest (see [Schrödinger Quantum Corrections on page 125](#)). Therefore, it is advantageous to simulate a slice through the middle of the channel as this is much faster to simulate, particularly when solving the Poisson–Schrödinger equation.

Previously, you did this by setting up the reduced structure manually and setting `remove_source_drain=on`. This required setting up a new input file to describe this reduced structure. You can use the `autoslice` parameter to automate this process as follows:

```
simulation autoslice=on
```

You must set up the device structure and input file as when simulating the entire device. The entire structure is read by Garand and initialized. A cross-sectional slice through the middle of the gate, normal to the channel direction, is then extracted and mapped onto a 1 nm wide slice (Garand requires a 3D simulation domain), and the subsequent simulations run with this slice as the solution domain. This is illustrated for a nanowire transistor in [Figure 9](#).

*Figure 9 Example nanowire transistor with resultant simulation domain obtained using `autoslice` parameter*



#### Note:

Since the source and drain regions are removed, Garand enforces a drain bias of  $V_d = 0$  V.

## Chapter 2: Importing Device Structures

### Structural Modifications

The autoslice is located at the midpoint of the gate in the channel direction. By default, the midpoint is the point that is halfway between the minimum and maximum extents of the gate in that direction. If the gate structure is in some way asymmetric, then this might not necessarily coincide with the middle of the channel. If this is the case, then there are alternative ways in which the autoslice location can be defined as follows:

```
simulation autoslice_position= gate_middle | gate_mean | <position>
```

where:

- `gate_middle` is the default behavior as described.
- `gate_mean` calculates the mean position of each mesh point within the gate and uses the component corresponding to the channel direction to define the autoslice position.
- `<position>` is an explicit location, in input units, along the channel direction at which to perform the autoslice.

When running an autoslice simulation, Garand also automatically generates output cutlines of the majority carrier density at positions in the structure that should be appropriate for calibration of the inversion layer charge density (see [Autocutlines on page 171](#)).

---

## Setting a Maximum Doping Limit

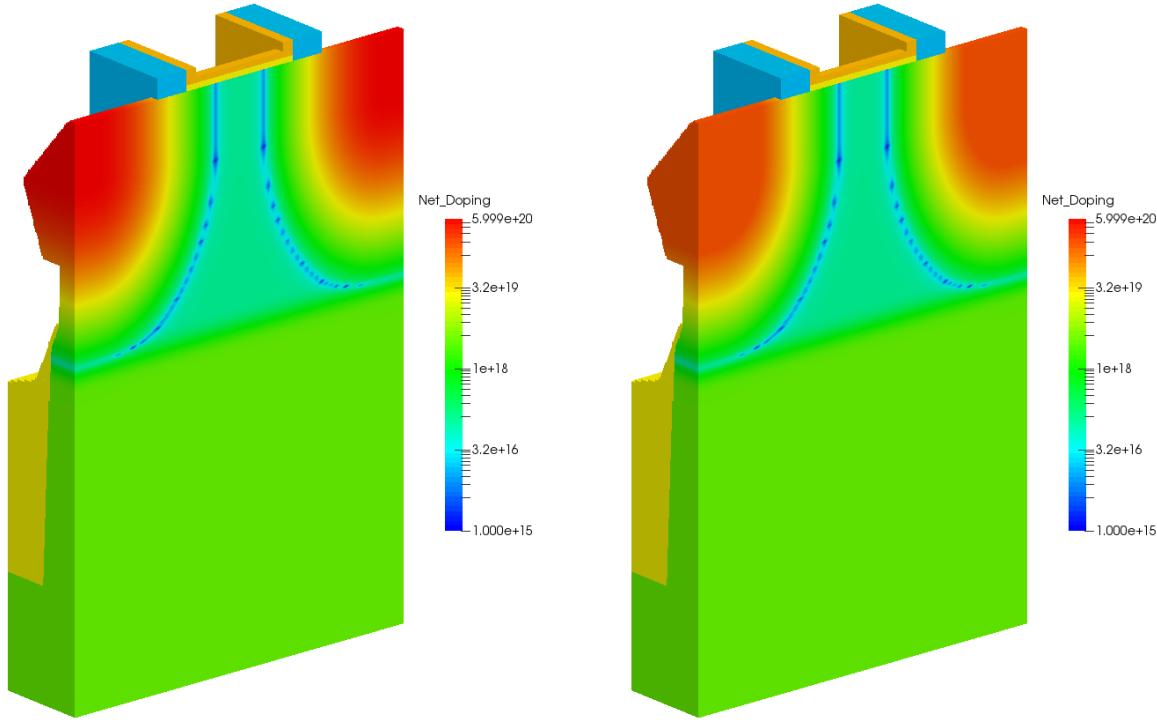
You can set a limit for the doping in simulated structures. If the doping concentration in an imported structure is greater than the specified limit, then the concentration value is set to the limiting value. This is achieved with the following command:

```
doping max_doping=<float>
```

The following example limits the doping in the simulated structure to  $2\text{e}20 \text{ cm}^{-3}$ :

```
doping max_doping=2e20
```

**Figure 10** FinFET example with peak source/drain doping of  $6\text{e}20 \text{ cm}^{-3}$  for (left) default structure and (right) with  $\text{max\_doping}=2\text{e}20 \text{ cm}^{-3}$



## Eroding the Source and Drain Contacts

The `erode_sd` parameter erodes a structure from the source and drain contacts into the semiconductor, converting the semiconductor material into a contact where particles will not be included in the Monte Carlo simulations.

A doping concentration is specified in the input file, and any mesh elements connected to the source/drain contacts that contain a node with doping concentration greater than the specified level are converted into part of the contact region. The command is:

```
structure erode_sd=<float>
```

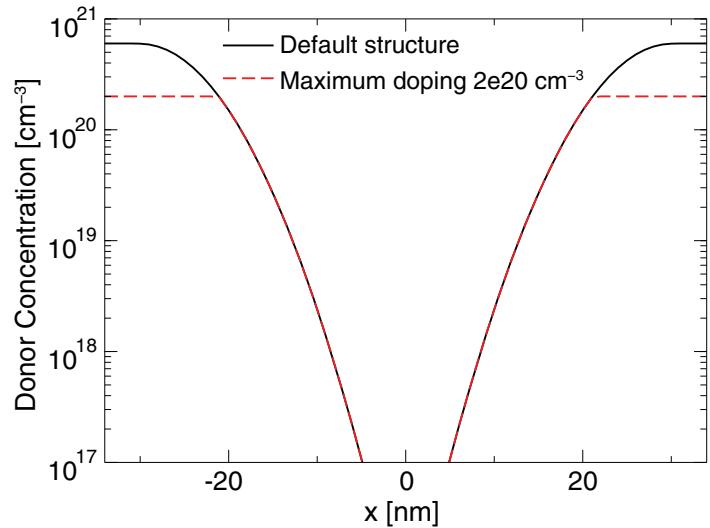
The following example starts at the source/drain contacts and erodes the structure converting any mesh element with doping greater than  $2\text{e}20 \text{ cm}^{-3}$  into part of the contact (see [Figure 11](#)):

```
structure erode_sd=2e20
```

## Chapter 2: Importing Device Structures

### Structural Modifications

Figure 11 Donor concentration in a cutline from source to drain in the FinFET in Figure 10 for default structure and  $\text{max\_doping}=2\text{e}20 \text{ cm}^{-3}$



The metallurgical contact, where boundary conditions are applied, moves to the new interface between the expanded contact region and the semiconductor, as illustrated in Figure 12.

To prevent the erosion function from removing too much of the structure, which can occur if there is a path of high doping that extends well into the device, you can limit the extent of the erosion so it remains within a bounding box specified for the source and drain contacts in the contact specification. Use the following command:

```
structure restrict_erode_sd=on
```

## Chapter 2: Importing Device Structures

### Structural Modifications

Figure 12 FinFET example with peak source/drain doping of  $6\text{e}20 \text{ cm}^{-3}$  for (left) default structure and (right) with source/drain eroded to a doping concentration of  $2\text{e}20 \text{ cm}^{-3}$

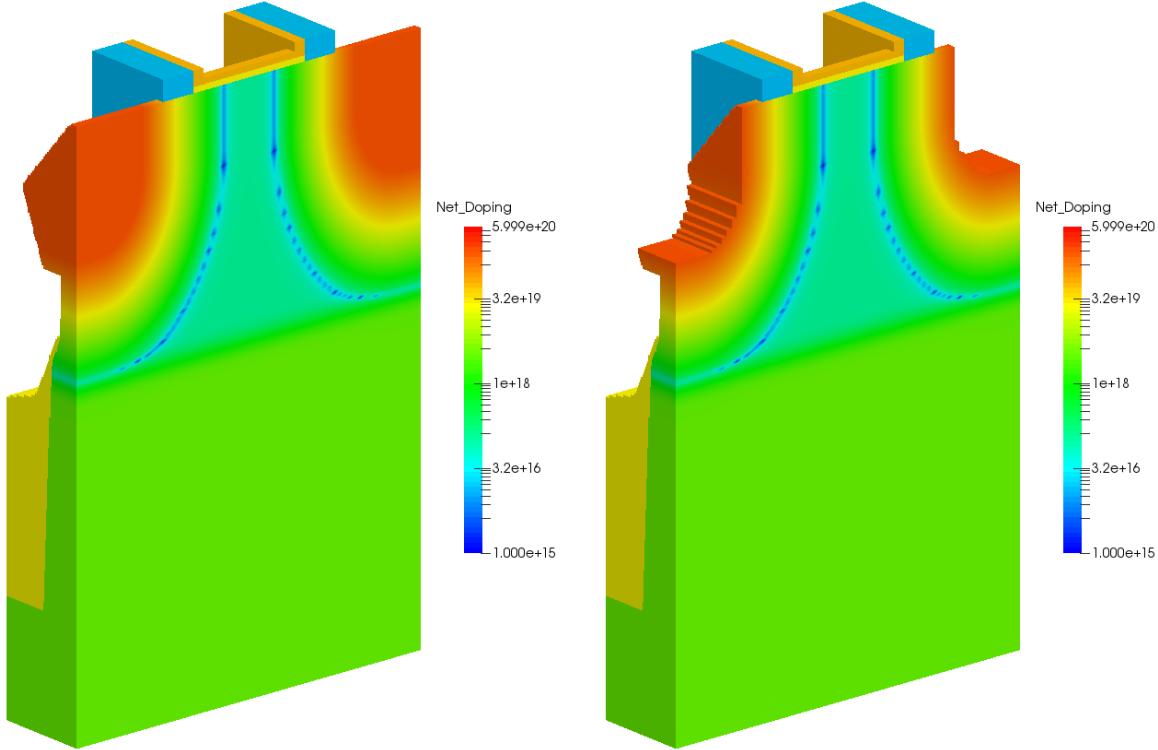
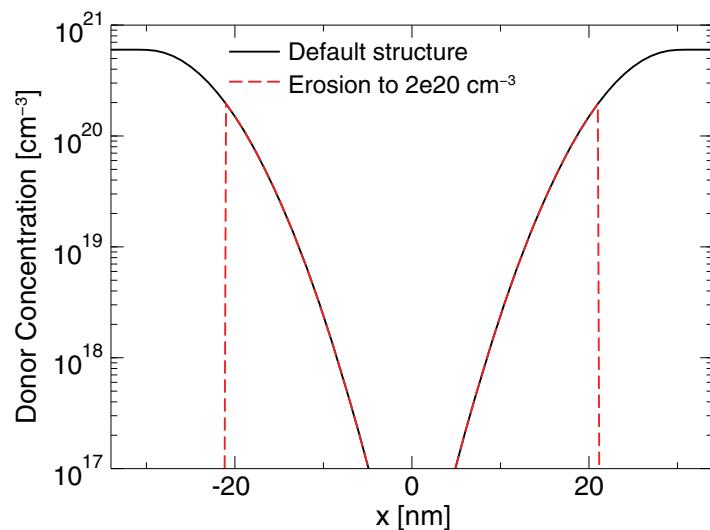


Figure 13 Donor concentration in a cutline from source to drain in the FinFET shown in Figure 10 for default structure and  $\text{erode\_sd}=2\text{e}20 \text{ cm}^{-3}$



## Adding a Uniform Fixed Charge

You can add a region of uniform fixed charge to the simulation structure by using the `structure add_charge` command (see [Adding a Uniform Fixed Charge on page 904](#)).

The `density` parameter specifies the volume density of charge to be added. This density is signed, so a positive density adds a positive charge and a negative density adds a negative charge.

You can specify an overall bounding box with the `xmin`, `xmax`, `ymin`, `ymax`, `zmin`, and `zmax` parameters. Then, the charge is added only to mesh cells that fully lie within this box.

To specify a list of materials within the bounding box to which the charge should be added, you can provide a comma-separated list of material names using the `material` parameter.

To restrict the charge to specific regions within the bounding box, you can provide a comma-separated list of region names using the `region` parameter. If `material` has also been specified, then the regions listed must contain one of the materials listed in `material`.

In summary, for a mesh cell to have the specified uniform charge added to it, it must be fully within the bounding box, contain one of the materials listed in `material` (if specified), and be within one of the regions listed in `region` (if specified).

---

## Alloy Fractions

This section discusses alloy fractions.

---

### Importing an Alloy Fraction

When importing a structure from a TDR file, Garand tries to import the `xMoleFraction` field, which represents the alloy fraction,  $x$ , in alloy materials such as  $\text{Si}_{1-x}\text{Ge}_x$ ,  $\text{In}_{1-x}\text{Al}_x\text{As}$ , and  $\text{In}_{1-x}\text{Ga}_x\text{As}$ .

For SiGe, Garand supports full spatial variation in material parameters. Therefore, each mesh node can have a different value of `xMoleFraction` and that alloy fraction can affect the material parameters at that mesh node. This results in a smooth variation in material parameters.

You can deactivate importing `xMoleFraction` with the command:

```
structure xMoleFraction=off
```

If you deactivate spatial variation of material parameters, then the treatment of the importing alloy fraction is different. Depending on the material defined in a particular mesh cell (for example, SiGe, InAlAs, or InGaAs), Garand uses the value of `xMoleFraction` imported with

the structure to allocate a specific fraction of the given alloy material. Traditionally, Garand has handled alloy materials by having separate materials defined for each 10% fraction of the alloy material. Therefore, the value of `xMoleFraction` used would be rounded to the nearest 0.1 and that fraction of the material would be assigned to the mesh.

For example, if the material specified for the mesh cell is SiGe and the value of `xMoleFraction` is 0.32, then `xMoleFraction` is rounded to the nearest 0.1 fraction (that is, 0.3) and the material assigned to the mesh cell is  $\text{Si}_{0.7}\text{Ge}_{0.3}$ . In Garand, alloy materials are referenced with the fraction expressed as a percentage, so the name of the material used in this case would be `Si70Ge30`. For a list of all Garand material names, including alloy fractions, see [Appendix A on page 842](#).

For  $\text{Si}_{1-x}\text{Ge}_x$ , you can change the default mapping by using the following command:

```
structure define_sige ge_x_min=0.0 ge_x_max=1.0 mat=Si60Ge40
```

This command allocates all fractions to  $\text{Si}_{0.6}\text{Ge}_{0.4}$ . The bounds can be altered to limit the number of  $\text{Si}_{1-x}\text{Ge}_x$  materials included in a simulation, which is particularly useful for pFET simulations where it is preferable to limit the number of semiconductor materials, to avoid excessive memory usage due to band-structure storage.

---

## Modifying Alloy Material Properties

You can modify the material parameters for alloy materials in the Garand input file in a similar way to non-alloy semiconductors such as silicon and germanium. However, some parameters in alloy materials are derived by interpolation between parameters of the base materials and, for these parameters, an interpolation method must be provided (see [Interpolation Methods on page 301](#)).

### Silicon Germanium

If the material in a region in a TDR file is `SiliconGermanium`, then it is imported to Garand as `SiliconGermanium`, even if `xMoleFraction=0` or is not present in the file. Therefore, when selecting mobility models or changing material parameters, these must be set for the `SiliconGermanium` material.

The following example selects the Philips unified mobility model for hole mobility in `SiliconGermanium`:

```
material SiliconGermanium.valence.mobility.bulk philips
```

If a constant value of a material parameter must be used for all fractions of `SiliconGermanium`, then this can be set in the same way as for a unary material.

## Chapter 2: Importing Device Structures

### Alloy Fractions

The following example sets the density gradient mass in the x-direction to 0.15 for all values of `xMoleFraction` (from silicon to germanium) within regions of the material `SiliconGermanium`:

```
material SiliconGermanium.conduction.dgx 0.15
```

Note, however, that this does not change the value in regions where the material is defined explicitly as silicon or germanium.

To define material parameters that vary with `xMoleFraction`, it is easier to use the piecewise linear specification where a value can be specified for a particular fraction of SiGe, and the values in between are interpolated with a linear interpolation. For example, the following commands set up the value for electron affinity (that is, the energy of the conduction band edge, `E`). Here, it is specified in 10% fractions from 0.0 to 1.0 and, for fractions in between these 10% definitions, it is interpolated linearly between the two values on either side:

```
material SiliconGermanium.conduction.E xMoleFraction 0.0 piecewise 4.05  
material SiliconGermanium.conduction.E xMoleFraction 0.1 piecewise 4.029  
material SiliconGermanium.conduction.E xMoleFraction 0.2 piecewise 4.021  
material SiliconGermanium.conduction.E xMoleFraction 0.3 piecewise 3.998  
material SiliconGermanium.conduction.E xMoleFraction 0.4 piecewise 3.989  
material SiliconGermanium.conduction.E xMoleFraction 0.5 piecewise 3.984  
material SiliconGermanium.conduction.E xMoleFraction 0.6 piecewise 3.938  
material SiliconGermanium.conduction.E xMoleFraction 0.7 piecewise 3.887  
material SiliconGermanium.conduction.E xMoleFraction 0.8 piecewise 3.832  
material SiliconGermanium.conduction.E xMoleFraction 0.9 piecewise 3.836  
material SiliconGermanium.conduction.E xMoleFraction 1.0 piecewise 3.92
```

For efficiency, when parameters are defined based on an imported alloy fraction field, Garand stores and reuses previously calculated parameters. The resolution used to store these parameters is 0.01, but it can be modified to make it coarser or finer, which can affect both the runtimes and the accuracy of simulations. The syntax to modify this is:

```
structure mole_fraction_interval = 0.001
```

When spatially varying parameters are deactivated, the fixed fraction material definitions (for example, `Si70Ge30`) obtain their parameters in the same way, so these example parameter definitions will be applied to each discrete material created.

Where a definition is provided with no specific mole fraction, it will be applied across all fractions. For example, the following commands set the orientation for all  $\text{Si}_{1-x}\text{Ge}_x$  materials in the simulation:

```
material SiliconGermanium.crystal.y 1 1 0  
material SiliconGermanium.crystal.x 0 0 1
```

Prior to Version N-2017.09, you could modify  $\text{Si}_{1-x}\text{Ge}_x$  materials by addressing the material name directly. For example:

```
material Si80Ge20.permittivity 10.0
```

This behavior can be activated by using the following command:

```
material <material>.parameters fixed_fraction
```

In this case, `<material>` is the name of the specific fixed fraction (`Si70Ge30`, for example).

## Other Alloys

For materials defined in 10% fractions, you can change the material parameters for a specific alloy fraction material (for example, `In50Al50As` for  $In_{0.5}Al_{0.5}As$ ) or simultaneously change the material parameters for all fractions of an alloy material. The following example changes the permittivity of `In50Al50As` to 12.0:

```
material In50Al50As.permittivity 12.0
```

No other InAlAs fraction is affected in this case.

To modify the mole fraction of a given alloy material, you can use the command:

```
material In50Ga50As.x_fraction 0.47
```

This command alters the `In50Ga50As` material to be  $In_{0.53}Ga_{0.47}As$ .

### Note:

Redefine alloy materials only to within 5% either side of the starting value to ensure the interpolation of the parameters is accurate. If the redefinition is greater than 5%, then a warning is issued. A redefinition above 10% terminates Garand with an error as the interpolation might not be accurate at this point. Redefining the fraction to 0.00 or 1.00 returns the parameters for the semiconductors used to form this alloy.

To modify all fractions of an alloy material, use the generic name (such as `InAlAs` or `InGaAs`) and Garand automatically applies the parameter change to all fractions of the material, including the base materials.

The following example specifies Masetti as the bulk electron mobility model to use for all fractions of InGaAs (from InAs to GaAs):

```
material InGaAs.conduction.mobility.bulk masetti
```

If the material parameter being modified requires an interpolator for alloy materials, then the interpolator to use must be specified as it would be for a specific fraction. The interpolator will be ignored when modifying the base material parameters, but it will be used for the fractions in between.

## Stress and Strain

This section discusses different aspects of stress and strain.

---

### User-Specified Stress or Strain

You can specify stress or strain in the input file using the `strain` command. This can be uniaxial or biaxial, or a full stress or strain tensor can be specified. For the input commands to specify this, see [Material Strain on page 285](#).

The resultant strain tensor for each material will modify the material properties that are used in the drift-diffusion simulation. If a strain-dependent mobility model is activated in the drift-diffusion simulation (see [Strain-Dependent Mobility Models on page 334](#)), then this strain tensor will also be used in the mobility model.

---

### Importing a Stress Tensor

Garand can import a stress tensor from TDR files and assumes that the stress tensor is stored in a tensor field called `stress`, which contains the following components:

- `stress-XX`
- `stress-YY`
- `stress-ZZ`
- `stress-XY`
- `stress-XZ`
- `stress-YZ`

Based on this imported stress tensor and a specified crystal orientation of the device structure, a resultant strain tensor will be derived. The effect of this strain on the material band structure and derived parameters is evaluated at each node in the simulation mesh. The models used to modify the band structure are described in [Material Strain on page 285](#).

**Note:**

This procedure can be computationally intensive and will slow down the initialization of simulations. By default, the impact of stress on the effective mass is neglected, but it can be activated using the following command:

```
material <material>.band>.strain_mass on
```

## Chapter 2: Importing Device Structures

### Stress and Strain

To activate the inclusion of strain effects from an imported stress tensor, specify the following command in the Garand input file:

```
strain import=on
```

To avoid the effects of artificially high “hot spots” of stress, there is a hard limit imposed on the maximum stress allowed in the simulation. The default is  $4 \times 10^9$  Pa, which you can modify by using the following command:

```
structure max_stress=<float>
```

where <float> is the maximum absolute value of stress allowed in the structure in pascals [Pa].

One effect of very high stress can be to reduce the band gap. To restrict any bandgap reduction so the band gap does not become zero (or even negative), there is a minimum limit imposed on the band gap. By default, this minimum limit is 0.1 eV, which you can modify by using the following command:

```
structure min_eg=<float>
```

where <float> is the minimum band gap limit in eV.

For example, to set the limit to 0.05 eV, specify:

```
structure min_eg = 0.05
```

For additional parameters associated with this command that apply only to Monte Carlo simulations, see [Spatially Varying Material Properties on page 228](#).

The effect of strain on carrier mobility can be included by activating a strain-dependent mobility model for the strained material (see [Strain-Dependent Mobility Models on page 334](#)).

If strain effects are included and a stress tensor has been imported from a TDR file, then both the stress and strain tensors are written to the output TDR file.

# 3

## Simulation Setup

---

*This chapter describes how to set up a Garand simulation.*

### Simulation Type: Target Current Search

A target current search is one of the simulation types that can be selected by using the command:

```
simulation sim_type=target
```

In this mode of operation, Garand tries to find the gate bias that results in a specified drain current in the device. The primary application of this mode is to find the threshold voltage,  $V_t$ , of the device based on a given current criterion.

The current that is the target of this search is specified with the command:

```
simulation target_current=<float>
```

where the parameter value is the target current in A.

A Secant method is used to search for the gate voltage,  $V_{target}$ , that results in the target drain current. In this method, a line is projected through the currents obtained in the two latest  $V_{target}$  predictions, and the  $V_g$  at which this line hits the target current is considered as the next prediction for  $V_{target}$ . As this is mainly intended for finding  $V_t$ , it is assumed that the target current will be in the subthreshold region. For this reason, the line projection is done on  $\log_{10}$  of the current, as the current depends exponentially on the gate voltage in the subthreshold. The projected line should be approximately the same as the subthreshold slope of the device.

The target current search starts at the gate voltage specified by the `bias gate` command (see [Bias Conditions on page 98](#)). To project a line to the target current to determine the next prediction for  $V_{target}$ , an assumed subthreshold slope is used in this first instance. By default, the subthreshold slope is 70 mV/decade. If you have a better estimate of what the subthreshold slope should be in the device, then you can specify the value to use initially with the command:

```
simulation target_init_slope=<float>
```

## Chapter 3: Simulation Setup

Simulation Type: Target Current Search

To aid stability of the search algorithm, a maximum limit is placed on the slope of the projected line that is used to obtain the next  $V_{target}$  prediction. By default, this limit is 200 mV/decade. If the subthreshold slope of the simulated device is actually greater than this limit, then you should increase the limit above the value of that subthreshold slope; otherwise, convergence to the target current might be slow. The maximum slope limit in mV/decade can be set with the command:

```
simulation target_max_slope=<float>
```

As the search progresses, the change in  $V_g$  from one prediction of  $V_{target}$  to the next is monitored. When that change becomes less than a specified accuracy, the search stops and the latest prediction of  $V_{target}$  is reported as the final result of the search.

The accuracy, in volts, required for the search can be specified with the command:

```
simulation target_acc=<float>
```

The search also stops after reaching an iteration limit. By default, this limit is 10 iterations of the search algorithm. This can be changed with the command:

```
simulation target_iter_max=<integer>
```

If the iteration limit is reached without finding  $V_{target}$ , then Garand reports that the target has not been found. This usually occurs if the starting gate voltage is not close enough to the target gate voltage. If the starting gate voltage is too low, in the deep subthreshold, then the current might be extremely small, and the simulation might struggle to converge. In this case, it might take several iterations to reach a gate voltage that produces a reliable current from which the search algorithm can find the target. Increasing the iteration limit allows the search algorithm to find the target eventually, but choosing a closer starting voltage would result in a faster solution.

Likewise, if the starting gate voltage is too high, in the above-threshold region, then projection to the next prediction of  $V_{target}$  when based on log10 of the current is not reliable. It will take several iterations for the search to work its way back to the subthreshold, from which point, the search algorithm can operate reliably.

In general, even when starting under non-ideal conditions, the search algorithm will find the target eventually if given enough iterations. However, the search in these cases might take significantly longer than it would under better starting conditions.

The output from the target current search records the successive predictions for  $V_{target}$  at each iteration and the current produced with that gate bias. When the target is found, the final point should show a current very close to the target value.

## Bias Conditions

You can specify the applied bias on each of the drain, gate, source and substrate contacts, relative to ground, either in the input file or on the command line. Drain and gate biases must be specified. By default, source and substrate biases are assumed to be 0.0 V.

**Note:**

Garand uses the standard bias conventions for PMOS devices where the applied gate and drain biases are negative for standard operation. For compatibility purposes, to use the old Garand convention of positive biases for PMOS devices, specify the `--legacy` command-line option.

Parameters for the applied bias are set using the `bias` command (see [bias Command on page 848](#)):

```
bias <parameter>=<value>
```

Garand operates in different modes depending on the setting of the command `simulation sim_type=<string>` (see [Simulation Setup on page 43](#)).

---

## I–V Characteristic Modes

When you operate Garand in I–V characteristic mode, `simulation sim_type=idvd` or `simulation sim_type=idvg`, for the following parameters of the `bias` command:

- `drain` sets the drain bias conditions of the first point in the I–V curve.
- `gate` sets the gate bias conditions of the first point in the I–V curve.
- `source` sets the source bias conditions of the entire I–V curve.
- `substrate` sets the substrate bias conditions of the entire I–V curve.
- `delta` sets the change in bias at each point of the I–V curve. This applies to either the gate contact or the drain contact, depending on whether `sim_type=idvd` or `sim_type=idvg`.
- `ivpoints` sets the number of I–V points to simulate. Therefore, the I–V curve covers the range from `gate` to `gate + (ivpoints - 1) × delta` (assuming an  $I_d$ – $V_g$  curve).

Instead of specifying the number of voltage steps (`ivpoints`) and the change in voltage (`delta`), you can simply specify the voltage values you want to use.

When running an  $I_d$ – $V_g$  curve, providing a comma-separated list of gate voltage values for the `gate` parameter will run simulations at those applied gate biases.

## Chapter 3: Simulation Setup

### Bias Conditions

#### Note:

There must be no spaces between values in the list.

The following command runs a simulation with gate biases of 0.0, 0.1, 0.5, and 1.0 V at the drain voltage specified by the `drain` parameter:

```
bias gate=0.0,0.1,0.5,1.0
```

Similarly, when running an  $I_d$ - $V_d$  curve, you can provide a comma-separated list of drain voltage values for the `drain` parameter. For example:

```
bias drain=-0.01,-0.05,-0.2,-0.5,-1.0
```

This command runs a simulation for a PMOS device with drain biases of -0.01, -0.05, -0.2, -0.5, and -1.0 V at the gate voltage specified by the `gate` parameter.

You can also specify a list of drain bias points when performing an  $I_d$ - $V_g$  simulation and Garand will produce the  $I_d$ - $V_g$  characteristics for each drain bias in the list, and similarly for a list of gate bias points when running  $I_d$ - $V_d$  simulations.

The substrate bias can also be specified as a list, and I-V characteristics will be produced for each substrate bias given.

---

## Target Current Search Mode

When you operate Garand in target current search mode, simulation `sim_type=target` (see [Simulation Type: Target Current Search on page 96](#)), for the following parameters of the `bias` command:

- `drain` sets the drain bias conditions for which the target current should be found.
- `gate` sets the gate bias conditions from which the search should start.
- `source` sets the source bias conditions for which the target current should be found.
- `substrate` sets the substrate bias conditions for which the target current should be found.
- `delta` is ignored because the search algorithm determines the change in gate bias.
- `ivpoints` is ignored because the number of points simulated depends on the convergence of the search algorithm.

At each subsequent iteration of the search algorithm, the gate bias is updated to the latest prediction for the target gate bias,  $V_{target}$ .

## Statistical Variability Sources

Garand can evaluate the impact of several statistical variability sources on device characteristics. These sources can be activated and defined in the input file, some of which have additional parameters that you must provide. These are set by using the [variability](#) command (see [variability Command on page 906](#)).

---

### Random Discrete Dopants

In the fabrication of semiconductor devices, impurity ions are introduced using ion implantation and are subject to high-temperature annealing, resulting in inherently random discrete dopant (RDD) distributions. Random dopants are introduced in Garand through a rejection technique based on the continuous doping profile coming from a standard TCAD process simulation.

To represent statistically the ‘average’ TCAD doping profile, each silicon lattice site within the device is visited and a dopant is placed based on a calculated probability that depends on the nominal continuous doping concentration at that point [1].

As the placement of discrete dopants depends only on the nominal doping profile, no additional parameters are required when activating the simulation of RDD. It is possible to specify whether all doping is discrete, or solely acceptors or donors. The generated random dopant positions will be written as particle data to the output TDR file.

For details about the parameters specific to RDD, see [Random Discrete Dopants on page 906](#).

By default, discrete doping is used everywhere in the simulation domain except at nodes that form part of the contacts. The discrete doping region can be restricted to a specific part of the device structure by providing a bounding box given by `xmin`, `xmax`, `ymin`, `ymax`, `zmin`, and `zmax`. It is not necessary to specify all of these parameters because, by default, the bounding box fills the *entire* simulation domain, with the default values for these parameters being the minimum or maximum extent of the simulation domain in the respective directions.

**Note:**

For large device structures, reduce the size of the discrete doping region as initializing a random dopant distribution can take time if the simulation domain is large.

Garand also includes a model that can vary channel mobility based on the number of discrete dopants in the region (see [Random Dopant Mobility Variation on page 159](#)).

## RDD From Separate Dopant Species Fields

When generating RDD, it is possible to consider each dopant species separately and to specify individual dopant species that should be considered as discrete dopants. This method of generating RDD dopant profiles produces different dopant positions from the method that only considers whether the dopants are acceptors or donors, so it must be activated explicitly, if required, by using the input file command:

```
variability RDD separate_species=on
```

By default, all dopant species are converted to discrete dopant profiles. To specify particular dopant species fields to use for RDD, use the input file commands:

```
variability RDD acceptor_fields = <string>
variability RDD donor_fields      = <string>
```

where <string> are comma-separated lists of acceptor and donor dopant fields. For example:

```
variability RDD acceptor_fields = BoronActiveConcentration
variability RDD
    donor_fields=ArsenicActiveConcentration,PhosphorusActiveConcentration
```

### Notes

- If you do not specify `acceptor_fields`, then ALL acceptor dopant fields are converted to RDD, and likewise for `donor_fields`. This specification acts restrictively to limit the fields made discrete to only those specified in the corresponding list. Therefore, the default behavior, if no species fields are specified, is as before, where all donor and acceptor doping is made discrete, although the generated dopant positions will be different from previously.
- The choice of whether acceptors, or donors, or both are converted to RDD is still controlled by the following command:

```
variability RDD dopants = all | acceptors | donors
```

Therefore, if only acceptors should be discrete, then the donor doping will remain continuous, even if `donor_fields` is specified, and likewise for acceptors.

- Any field specified with these commands must have been imported from the TDR file, either as one of the default dopant fields or in the list of fields specified by users. If the doping field was not imported, then Garand stops with an error.

If extra doping is obtained from the `DopingConcentration` field, as described in [Extra Doping From the DopingConcentration Field on page 65](#), then it is not intrinsically included in any dopant species fields. As Garand can generate random discrete doping on a species-by-species basis, the extra doping would not be included in the discrete doping and would remain as continuous doping. To avoid this problem, Garand generates additional “artificial” species fields (`ExtraAcceptorConcentration` and `ExtraDonorConcentration`)

## Chapter 3: Simulation Setup

### Statistical Variability Sources

if required, to contain any extra donor or acceptor doping obtained from the DopingConcentration field. These can be treated like any other species field when explicitly specifying a list of species fields to be made discrete. For example:

```
variability RDD donor_fields=
    ExtraDonorConcentration,ArsenicActiveConcentration
```

## RDD in Polysilicon Gates

By default, random discrete dopants are generated in polysilicon gates. You can control this behavior from the Garand input file by deactivating RDD in polysilicon gates as follows:

```
variability RDD include_poly=off
```

## Outputting Positions of Random Discrete Dopants

Random discrete dopants are written as particle data to the output TDR file, so the positions of the dopants can be visualized. To output the actual positions of each discrete dopant, the RDD positions can be written to a text file.

To write the dopant positions into a file, include the command:

```
variability RDD write_positions = on
```

The file will be written to the output directory with the file name:

```
<experiment>-Dopant-Positions-<device_number>.dat
```

This file has four columns:

- The first column is the name of the dopant field that contains the particular dopant on that line.
- The next three columns are the x-, y-, and z-coordinates of the dopant in nanometers.

## Importing Positions of Random Discrete Dopants

Rather than allowing Garand to generate random dopant locations based on the continuous doping profile, you can import the positions of discrete dopants that come, for example, from a kinetic Monte Carlo model of the ion implantation process.

This is done using the `import` option. Garand supports the following file formats for imported dopant positions:

- Plain text file with three columns
- Kinetic Monte Carlo defects file written by Sentaurus Process

### Plain Text File With Three Columns

This format of discrete dopant position file should have one line for each dopant to be added containing the x-, y-, and z-coordinates of the dopant in specified units. Any line that does not contain three numbers is ignored. Acceptor and donor positions must be in separate files as each file will be treated as containing a list of either acceptor positions or donor positions.

To import dopant positions from a plain text file, use the input file command:

```
variability RDD import species=<string> file=<string> units=<string>
```

For descriptions of the parameters, see [Importing Positions of Random Discrete Dopants on page 908](#).

For example:

```
variability RDD import species=acceptors file='B.txt' units=um  
variability RDD import species=acceptors file='In.txt' units=um  
variability RDD import species=donors file='As.txt' units=um  
variability RDD import species=donors file='P.txt' units=um
```

### Kinetic Monte Carlo Defects File

When running a kinetic Monte Carlo (KMC) implantation simulation in Sentaurus Process, you can write the positions of each implanted ion to a file. This file can be read by Garand to extract the discrete dopant positions for an RDD simulation. To write such a file, include a line of the following form in the Sentaurus Process command file:

```
kmc defects.write= Defects.txt defectname= PointDefect \  
materialname= Silicon
```

For more information, see the *Sentaurus™ Process User Guide*, Adding and Obtaining Defects in Simulations: add, defects.add, and defects.write.

This file contains the discrete dopant positions (tagged as PointDefects) in the materials specified, labeled by the impurity atom (that is, As, P, B, In), as shown here:

PointDefect	As	-14.548530	2.381407	1.855797
PointDefect	As	-14.257627	1.564710	2.044811
PointDefect	P	0.346941	-2.112056	-0.817567
PointDefect	B	1.147740	-2.388342	0.703612

The three numbers on each line are the x-, y-, and z-coordinates of the dopant in **nanometers**.

To ensure that the KMC dopant positions are output in the same coordinate system as the device structure, you must also include the following command in your Sentaurus Process simulation command file:

```
math cord.-zyx
```

## Chapter 3: Simulation Setup

### Statistical Variability Sources

To import dopant positions from a KMC defects file, use the input file command:

```
variability RDD import species=<string> file=<string> field=<string>
```

For descriptions of the parameters, see [Importing Positions of Random Discrete Dopants on page 908](#).

This differs from the command for the plain text format in that it has the `field` parameter that identifies the impurity atom field to read, that is, As, P, B, and In. It is the inclusion of the `field` parameter that tells Garand that the file is a KMC defects file.

#### Note:

Only the positions identified by `field` are included in the simulation, based on this input file command.

Specify one `RDD import` command for each different field to read.

For example:

```
variability RDD import species=donors      file='Defects.txt' field='As'  
variability RDD import species=donors      file='Defects.txt' field='P'  
variability RDD import species=acceptors   file='Defects.txt' field='B'
```

These commands read the fields labeled As and P in the file (arsenic and phosphorus) and store them as donor positions, and the field labeled B (boron) and store it as acceptor positions. Units have not been specified as the KMC defects file always contains the positions in nm.

#### Notes

- You can specify multiple `variability RDD import` commands in the input file.
- The units specified in one such command apply *only* to the file specified in that command and must be specified for each file if the units are not nm.
- You can specify multiple files containing discrete dopant positions, even for the same species type.
- The `status` parameter still applies to imported positions as follows:
  - If `status=off`, then no random dopants are applied.
  - If `status=on` and `dopants=acceptors` or `dopants=donors`, then only the specified dopant type are applied and the other dopant type retains a continuous doping distribution.
  - If `dopants=all`, then both imported acceptors and imported donors are applied.

## Chapter 3: Simulation Setup

### Statistical Variability Sources

- If only one type of imported dopant (acceptors or donors) is specified in the input file, then discrete doping applies only to that type of dopant, even if you specify `dopants=all`.
- Any RDD bounding box specified also applies to imported dopants.

---

## Line Edge Roughness

Line edge roughness (LER) is mainly due to the macromolecular structure of the photoresist and the corpuscular nature of light. LER is introduced in Garand through randomly generated lines that can be applied, for example, to the gate edges.

The random lines used to modify the device structure are generated using a Fourier synthesis technique and are characterized by two parameters:

- The root mean square (RMS) amplitude of the line,  $\Delta$ , determines the magnitude of the roughness, with the quantity usually referred to as the LER being defined as  $3\Delta$  (this is analogous to  $3\sigma$  of a normal distribution, where  $\sigma$  is the standard deviation).
- The longitudinal correlation length,  $\Lambda$ , controls the rate at which the random lines vary along their length, with a small value resulting in fast variations and a larger value leading to more long-scale roughness.

To add LER to an arbitrary imported structure, the variability type `LER` is used. All the options for this particular roughness specification **must** be supplied in the same command line in the input file. This is because LER can be applied in multiple directions simultaneously.

LER is characterized by two random lines that model the roughness on either end of the gate. The starting point is to specify a point in one direction that defines a plane normal to which the structure will be modulated to follow the roughness. This would typically be the midpoint of the gate in the channel direction.

This is shown in [Figure 14](#) where a plane is defined at  $x = 0.0$  nm. The direction in which the roughness propagates must also be specified using the `dir` parameter. This will be in one of the two directions that form the midpoint plane.

In the example of [Figure 14](#), this can be either the y- or z-direction. An example command to set up the LER shown in [Figure 14](#) would be, for the upper option:

```
variability LER status=on x=0.0 dir=y rms=<float> corr=<float>
```

and for the lower option:

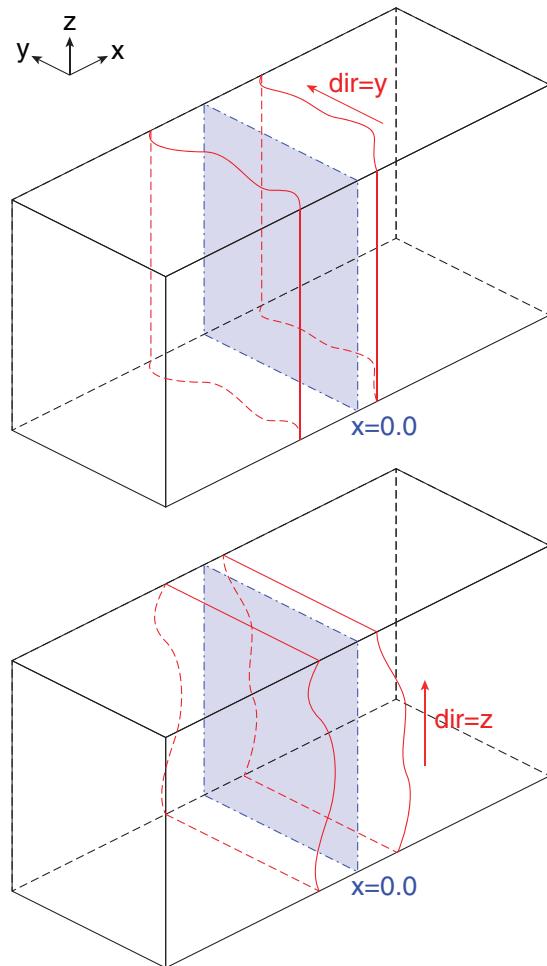
```
variability LER status=on x=0.0 dir=z rms=<float> corr=<float>
```

with the assumption that `rms` and `corr` must also be specified in order to have roughness patterns.

## Chapter 3: Simulation Setup

### Statistical Variability Sources

Figure 14 Specifying the midpoint and the direction of the roughness when applying LER to an arbitrary imported device structure



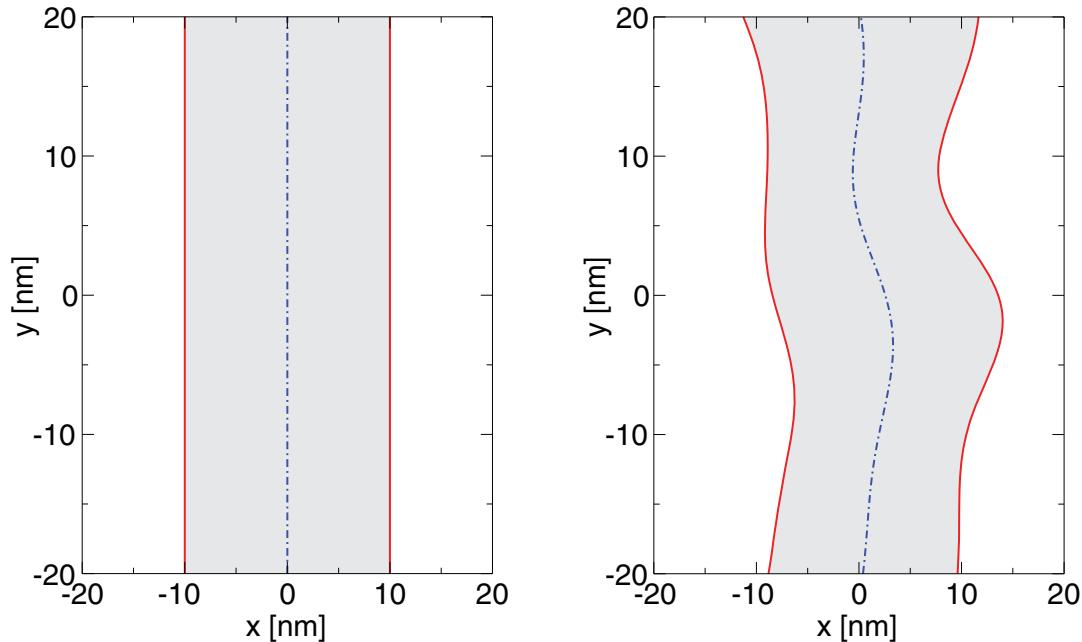
For details about the parameters specific to LER, see [Line Edge Roughness on page 909](#).

Two random lines are generated as previously described, with the RMS amplitude and the correlation length specified by the `rms` and `corr` parameters, respectively. The original midplane is modulated by a line that is the average of the two random lines, and the two roughness patterns are applied to either side of the modified midplane such that random line 1 modulates the structure on one side and random line 2 affects the structure on the other side as shown in [Figure 15](#).

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### Statistical Variability Sources

**Figure 15** Example of LER mapping from (left) uniform structure to (right) rough structure, where the specified LER midplane (dashed line) is mapped to the average of the two random lines, and either side of this middle line is moved by the rough line on that side



Modifying the midplane by the average of the two lines ensures that the device structure is symmetric about this point (assuming the uniform device structure was symmetric about the original specified midplane), which helps when dealing with doping profiles as described below.

Two other parameters available for LER in this case are `uniform` and `correlated`. The `uniform` parameter allows a simulation where the roughness patterns used are in fact uniform with a constant positive or negative value, which will uniformly move the gate edges outwards or inwards, respectively. Each gate edge is moved by the amount specified so, for example, `uniform=3.0` will increase the total gate length by 6 nm while `uniform=-3.0` will reduce the total gate length by 6.0 nm. The `correlated` parameter specifies correlated LER where the same roughness pattern is used on both gate edges.

As well as edge roughness with the given statistical properties (`rms` and `corr`), you can overlay line width variation (LWV) with a Gaussian distribution. This will move the device structure uniformly in or out from the midpoint plane depending on a random number generated from a Gaussian distribution with a given standard deviation. A positive random number  $R$  will move each side outwards by  $R/2$ , while a negative random number will move each side inwards by  $R/2$ .

To specify the standard deviation of the LWV, set the `lwv` parameter to the required standard deviation in nm. If no roughness is specified or `rms=0.0`, then the variation in line edge will

## Chapter 3: Simulation Setup

### Statistical Variability Sources

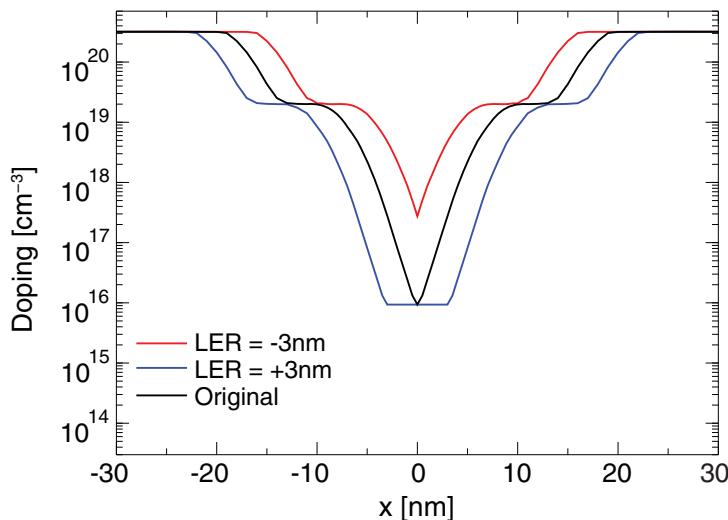
be uniform following the LWV specification. If edge roughness is included, that is,  $r_{rms} > 0.0$ , then the edge roughness will be superimposed on any line width variation coming from the LWV specification.

## Default Doping Profiles

As the device structure is modulated by the random lines, so the doping profiles must also move to follow the roughness on either end of the gate. For doping profiles that were implanted using the gate or spacer as a mask, such as source/drain implantations and halo implantations, this can be problematic as local changes in the gate length due to LER should increase or decrease the overlap of such implantations in the middle of the channel.

Without further consideration, the effect on the doping profiles of shorter or longer gate lengths is shown in Figure 16. The original profile (black line) is considered from either the source or drain end to the midpoint and moved either inwards, such that it is truncated at the midpoint (red line) or outwards, such that past the point that was originally the midpoint the doping remains constant as there is no information available beyond this.

Figure 16 Default behavior when LER reduces (red line) or extends (blue line) the gate length of a bulk MOSFET



## Reconstructed Doping Profiles

While this default behavior gives consistent and reliable doping profiles, it results in inaccuracies in the evaluation of LER effects as it cannot reproduce the correct  $V_t$  roll-off behavior that characterizes LER-induced variability, particularly when there are overlapping halo profiles. Garand provides a method to better approximate the varying overlap of doping profiles with varying gate length.

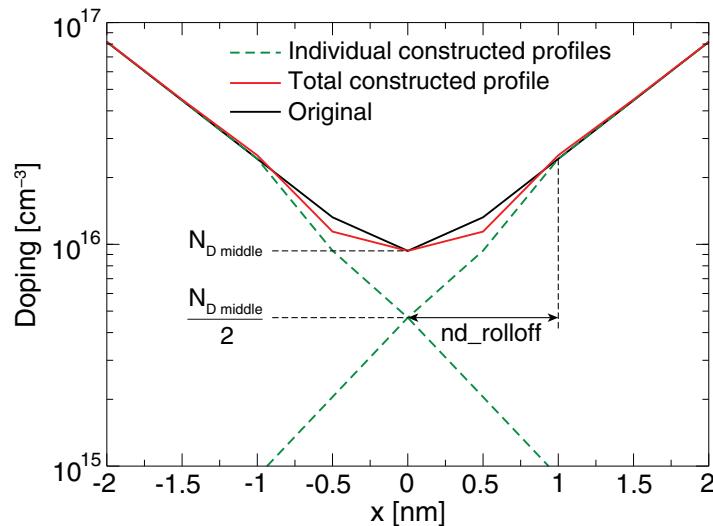
## Chapter 3: Simulation Setup

### Statistical Variability Sources

You can use this method when the doping in the middle of the channel (at the midpoint specified in the input file `variability LER` command) is the sum of two implantations: one from the source side and one from the drain side.

Assuming that the two implantations are symmetric, if the doping in the middle of the channel is  $N_{D\text{middle}}$ , then the doping concentration of each separate doping profile at this point is  $N_{D\text{middle}}/2$  as shown in [Figure 17](#).

*Figure 17 Method of projecting a single-sided doping profile past the middle of the channel*



By supplying a distance for `nd_rolloff`, Garand constructs a single-sided profile by considering the slope of the doping profile between the middle point, with doping concentration  $N_{D\text{middle}}/2$ , and the point that is `nd_rolloff` [nm] away from this point (or `na_rolloff` for an acceptor profile), and projecting this slope past the middle of the device. The separated source and drain doping profiles can then be moved following the rough line for their respective sides and summed to obtain a full doping profile for an effectively different gate length, as shown in [Figure 18](#). You can use the parameters `nd_rolloff` and `na_rolloff` to fine-tune the slope of the projected doping profile and, therefore, adjust the doping in the middle of the channel for parts of the device where the gate length is increased by the LER on both gate edges (see [Figure 19](#)).

#### Note:

Take care when using this method because it might produce unrealistic doping profiles if it is applied to inappropriate cases. It must be used only when doping decreases monotonically toward the midpoint. Testing using the `uniform` parameter for different resultant gate lengths and writing cutlines of the doping are useful to confirm that this method gives acceptable results (see [Exporting 1D Cutline Data on page 170](#)).

## Chapter 3: Simulation Setup

### Statistical Variability Sources

Figure 18 Illustration of the method to construct a single-sided doping profile by projecting the given profile past the middle of the device and then reconstructing the doping profile for a different gate length as the sum of two single-sided profiles

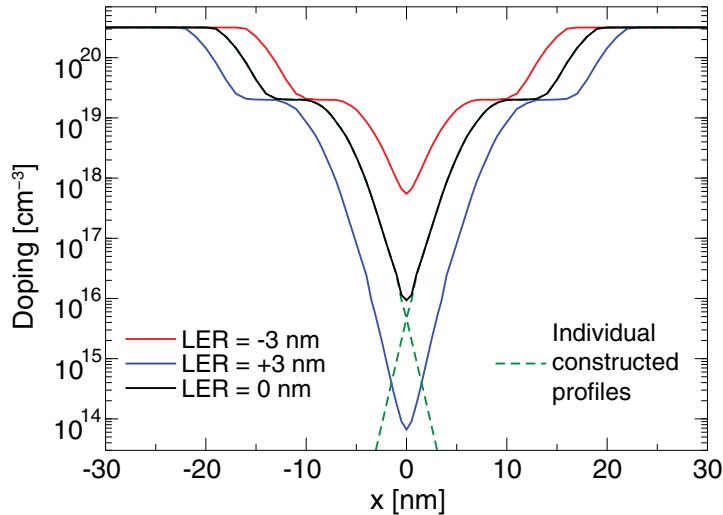
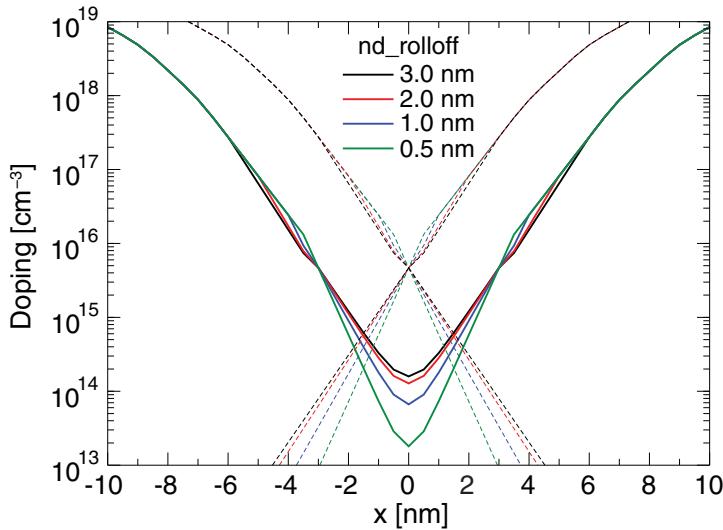


Figure 19 Effect of changing the roll-off starting point on the constructed doping profile with a 3 nm increase in the gate length at both the source and drain ends



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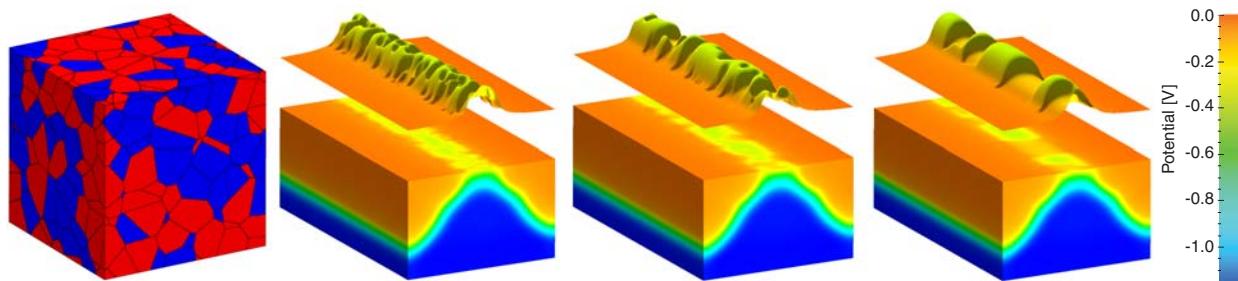
## Metal Gate Granularity

The polycrystalline nature of the metal gate is another potential source of statistical variability. Metal grains with different crystallographic orientations have different workfunctions at the metal–oxide interface, resulting in random variation of the local threshold voltage in the gate region [2][3][4].

Metal gate granularity (MGG) is introduced in Garand through the generation of random 3D grain patterns based on a 3D Voronoï tessellation, where the specified average grain size determines the average number of grains in the gate volume. For details about the generation of the grain pattern and the specification of average grain size, see [Generation of Laguerre–Voronoï Grain Pattern on page 113](#).

Each grain is assigned a random workfunction based on the probability and the number of different grains specified by users, as illustrated in [Figure 20](#) for two possible grain workfunctions. The workfunction of each grain is assigned based on the probability of a particular grain orientation occurring. The surface plot at the top of each figure shows the 2D potential at the oxide interface.

**Figure 20** (Leftmost) Example of grain pattern of a two-grain metal generated by a 3D Voronoï tessellation, with electrostatic potential in the 35 nm device (with 200 nm width) with TiN MGG as the sole source of variability and average grain diameter of (second left) 5 nm, (second right) 10 nm, and (rightmost) 20 nm



## Adding Metal Gate Grains

The number of different grain orientations for the gate metal depends on how many grains you define using the `add_grain` option. You must ensure that the sum of probabilities for the defined grains equals 1.0. Otherwise, Garand generates an error and stops the simulation.

For each grain orientation, you must provide two numbers: the first is the workfunction for that orientation (or an offset from the specified nominal workfunction) and the second is the probability (between 0.0 and 1.0) for that orientation to occur.

To add metal gate grains, use one of the following commands:

```
variability MGG add_grain workfunction=<float> probability=<float>
variability MGG add_grain wf_delta=<float> probability=<float>
```

For example, to specify the values of the workfunction to use explicitly:

```
variability MGG add_grain workfunction=3.88 probability=0.4
variability MGG add_grain workfunction=4.08 probability=0.6
```

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Alternatively, for example, to specify the workfunctions as an offset from the nominal workfunction:

```
variability MGG add_grain wf_delta=-0.12 probability=0.4  
variability MGG add_grain wf_delta=+0.08 probability=0.6
```

**Note:**

You cannot specify both `workfunction` and `wf_delta` in the same command.

The total sum of all the specified probabilities must be 1.0, and the weighted average (that is,  $(WF_1 \times P_1) + (WF_2 \times P_2) + \dots + (WF_n \times P_n)$ ) must be the nominal workfunction without MGG. When you specify `wf_delta`, the weighted average of the offset values must equal zero, for example,  $(-0.12 \times 0.4) + (0.8 \times 0.6) = 0.0$ .

For descriptions of the parameters, see [Metal Gate Granularity on page 910](#).

---

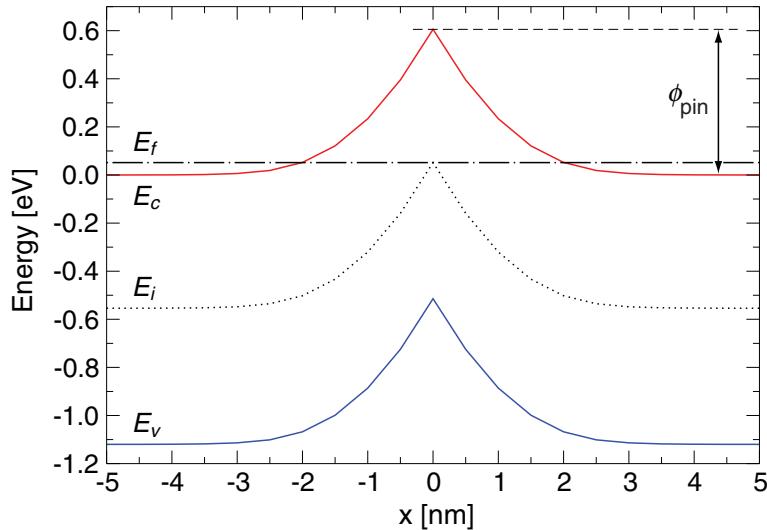
## Polysilicon Gate Granularity

The granularity of the polysilicon gate is an important source of statistical variability due to surface potential pinning along the grain boundaries. As with metal gate granularity, polysilicon gate granularity (PGG) is introduced in Garand through generation of random 3D grain patterns based on a 3D Voronoï tessellation, where the specified average grain size determines the average number of grains in the gate volume. Arbitrary surface potential pinning can be introduced at the grain boundaries. For details about the generation of the grain pattern and the specification of average grain size, see [Generation of Laguerre–Voronoï Grain Pattern on page 113](#).

For descriptions of the parameters, see [Polysilicon Gate Granularity on page 912](#).

[Figure 21](#) shows the effect of Fermi-level pinning on the band profiles in a highly n-doped polysilicon gate. In this case, the Fermi-level has been pinned at the middle of the band gap. You can use the `pinning` parameter to set the level at which the Fermi level must be pinned.

**Figure 21** Effect of Fermi-level pinning on the band profiles in a highly n-doped polysilicon gate; the average diameter of the polysilicon grains to be used can be specified using the diameter parameter



## Generation of Laguerre–Voronoi Grain Pattern

The previously described variability sources MGG (see [Metal Gate Granularity](#)) and PGG (see [Polysilicon Gate Granularity](#)) require a model of a polycrystalline grain pattern to be generated. This grain pattern is based on a 3D Voronoi tessellation.

You can control the size of the grains within the grain pattern by specifying an average grain diameter, in nm, with the `diameter` parameter, for the MGG and PGG variability models, respectively, as follows:

```
variability MGG diameter=<float>
variability PGG diameter=<float>
```

The volume of a sphere with this diameter is calculated and taken as the average volume of a grain. The average number of grains is then obtained by dividing the total volume to be filled by this average grain volume. This calculation assumes a perfect packing of the spheres into the volume. If you want to assume a less than perfect packing, then you can specify a packing density for the MGG and PGG variability models, respectively, as follows:

```
variability MGG packing_density=<float>
variability PGG packing_density=<float>
```

This parameter can take a value such that  $0.0 < \text{packing\_density} \leq 1.0$ . This factor scales the total volume to be filled with grains to account for the fact that the grain spheres do not fill the whole volume. This will result in a corresponding reduction in the average number of grains calculated.

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### Statistical Variability Sources

The actual number of grains generated in the structure, for a specific statistical device number, is taken randomly from a Poisson distribution whose expected value is the average number of grains, calculated as previously described. For each grain, a seed site is located randomly in 3D space within the bounding box of the volume to be filled, plus a buffer region around that box to account for grains that are only partially within the bounding box. This buffer region is included in the total volume when calculating the average number of grains.

Each mesh point in the grain region is designated as part of the grain associated with whichever seed site it is closest to, by a particular measure of *distance*. To obtain the standard Poisson–Voronoi pattern, the measure of distance used is the direct Euclidean distance between the mesh node and the seed site. In this case, in the resultant grain pattern, the relative standard deviation in grain volume is approximately  $\sigma_r = 0.42$  in all cases. This is smaller than the variation in grain volume observed in real polycrystalline grain structures [5].

To allow some variation in the standard deviation of grain volumes, in Garand, a Voronoi diagram in Laguerre geometry is used [5][6]. Here, a virtual sphere is centered on each seed site and the measure of distance to the site is the length of the tangent line to the surface of the sphere. If all the spheres have the same diameter, then you generate the standard Poisson–Voronoi diagram. However, if the diameters of the spheres vary, then the variation in grain volume,  $\sigma_r$ , can be increased.

The volumes of grains in a polycrystalline structure have been observed to follow a log-normal distribution. Therefore, a log-normal volume distribution is applied to the spheres used to generate the Laguerre–Voronoi diagram. The relative standard deviation of this distribution can be specified with the `volume_rsd` parameter for the MGG and PGG variability models, respectively, as follows:

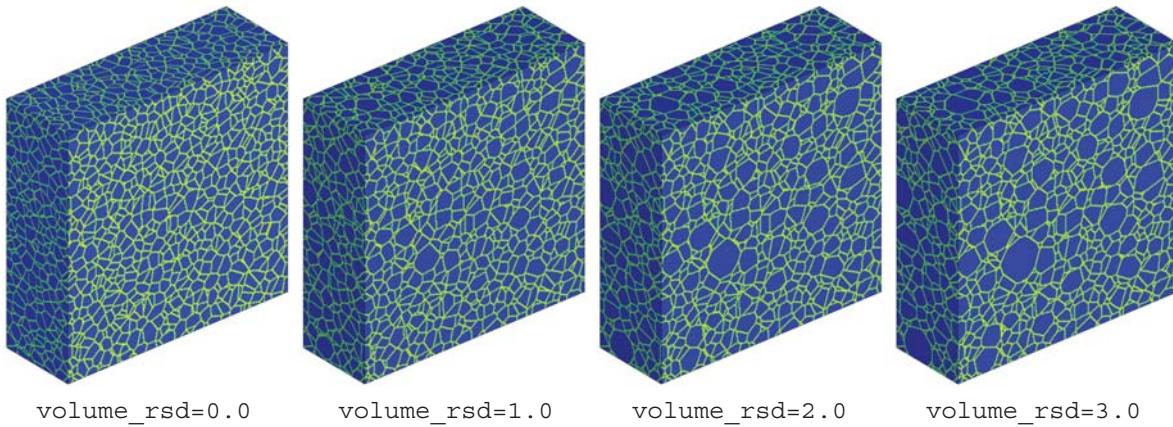
```
variability MGG volume_rsd=<float>
variability PGG volume_rsd=<float>
```

Figure 22 shows examples of grain patterns generated with a Laguerre–Voronoi diagram and with different values of `volume_rsd`.

#### Note:

The variation specified here is for the volume of spheres used in the Laguerre–Voronoi generation, not for the volume of the final polycrystalline grains. The volume of each grain is limited by the presence of neighboring grains and, therefore, the relative standard deviation in volume of the final grains is usually less than that specified for the Laguerre spheres.

**Figure 22** Example grain patterns produced with the Laguerre–Voronoi method; the relative standard deviation of the Laguerre sphere volumes is changed by setting the `volume_rsd` parameter



## Random Telegraph Noise

Random telegraph noise (RTN) can be caused by the trapping and detrapping of carriers in interface trap states. It is characterized by a discrete drop in current due to a trapping event and the return to the previous current level after detrapping. This can also be observed as an increase in threshold voltage.

The RTN variability model allows single or multiple discrete trapped charges to be added at a semiconductor–insulator interface. The simulation is run first without the trapped charge to provide the baseline characteristics, and then the trap is added and the simulation is rerun to provide the RTN response.

To control the application of RTN, use the command:

```
variability RTN <parameter>=<value>
```

For descriptions of the parameters, see [Random Telegraph Noise on page 913](#).

## Additional Random Trap

A single additional trap can be added randomly to an oxide interface within a defined bounding box. This trap is considered to be always filled.

To use the RTN variability model and to add this additional random trap, include the command:

```
variability RTN status=on
```

To restrict the random placement of the trap, a bounding box can be specified with the parameters `xmin`, `xmax`, `ymin`, `ymax`, `zmin`, and `zmax`. The placement of the random trap can

## Chapter 3: Simulation Setup

### Statistical Variability Sources

also be restricted to interfaces between specific semiconductor materials or regions, and specific oxide regions. See [Restricting the Interfaces at Which the RTN Trap Can Be Generated on page 116](#).

For a given statistical device number (specified with the `-d` command-line option), the added trap can be located at a different random position by changing the seed parameter:

```
variability RTN seed=<integer>
```

Starting with the seed specified with this command, within one simulation run, you can run a number of consecutive simulations where the seed is increased to produce a different random trap position. To specify the number of different random trap positions to simulate, you can set the `num_configs` parameter:

```
variability RTN num_configs=<integer>
```

## Adding Multiple Traps

The default behavior for the RTN variability model is to add one filled trap. This behavior can be modified with the command:

```
variability RTN expected_number=<integer>
```

The default for `expected_number` is 1 and, in this specific case, the previously described behavior of always adding one single trap is observed. However, if a positive integer other than 1 is set, then the actual number of traps added is selected randomly following a Poisson distribution, with the specified number of traps as the expected value of the distribution.

## Restricting the Interfaces at Which the RTN Trap Can Be Generated

You can specify the interfaces to which you want to limit the RTN trap. The first step is to specify which semiconductors the interface is on. This is done by specifying the semiconductor material with a comma-separated list of material names using the command:

```
variability RTN material=<string>
```

This can be refined further by specifying a list of semiconductor regions on whose insulator interfaces the trap could be placed:

```
variability RTN region=<string>
```

After the semiconductor side of the interface has been defined, by default, the trap could be placed at the interface between the defined semiconductor and any insulator. This can be restricted to the interface with a specific insulator by providing a comma-separated list of oxide regions with the command:

```
variability RTN oxide_region=<string>
```

**Note:**

Any bounding box that was specified for the RTN trap will still be respected

## Output

Output associated with the initial simulation without the RTN trap will produce files that use the provided experiment name as the beginning of the file name. For subsequent RTN simulations, files will have the string `_rtn-seed-<seed>` appended to the experiment name when setting the beginning of the file names, where `<seed>` is the numeric value of the seed used to randomly generate the positions of RTN traps in that simulation.

The positions of all RTN traps in a particular simulation are written as particle data to the output TDR file in the particle field `Garand/RTNTraps`.

---

## Workfunction Variation

As described in [Device Structure on page 45](#), the nominal uniform workfunction must be specified for a metal gate by using the command:

```
contact work_function=<float>
```

You can apply a Gaussian variation to this nominal workfunction so that, in a statistical ensemble of devices, each one will have a different uniform workfunction taken from a Gaussian distribution with a specified standard deviation. To specify the standard deviation of the variation, use the following command:

```
contact wf_sigma=<float>
```

where `wf_sigma` is the standard deviation of the Gaussian variation.

This workfunction variation can be used in combination with MGG. In this case, the offset in workfunction from the nominal workfunction in the different metal grains will then be applied relative to the new gate workfunction taken from the Gaussian distribution. Therefore, if the MGG has two grain orientations with workfunctions  $WF_{nom} - 0.12$  and  $WF_{nom} + 0.08$ , and the workfunction of the device changes from  $WF_{nom}$  to  $WF_{new}$ , then the workfunctions of the two metal grain orientations will then be  $WF_{new} - 0.12$  and  $WF_{new} + 0.08$ .

---

## Contact Resistance Variation

As described in [Contact Resistance on page 132](#), you can include source/drain resistance in the simulation by using one of the following commands:

```
contact resistance_lumped=<float>
```

```
contact resistivity_lumped=<float>
```

```
contact resistivity_distrib=<float>
```

You can also introduce statistical variation into the source and drain contact resistances. The variation is assumed to follow a Gaussian distribution with the mean value equal to the nominal resistance specified by one of these commands. Including a specification of a standard deviation (sigma) in the command, Gaussian variation with the given standard deviation will be applied:

```
contact resistance_lumped=<float> sigma_resistance=<float>
```

where the units of the resistance and standard deviation are ohms [ $\Omega$ ] or:

```
contact resistivity_distrib=<float> sigma_resistivity=<float>
```

where the units of the resistivity and standard deviation are  $\Omega \cdot \text{cm}^2$ .

Source and drain resistances will be chosen independently. The effective applied drain bias for a lumped resistance will then be  $V_{\text{Def}} = V_d - R_s I_s - R_d I_d$ .

---

## Statistical Reliability Modeling

It is becoming important to include statistical reliability information in process design kits (PDKs). Accurate statistical reliability information is crucial in defining the reliability criteria, and for reliability-aware statistical design. Negative bias temperature instability (NBTI) and positive bias temperature instability (PBTI) degradation are associated with the injection and trapping of carriers in defect states in the gate stack during circuit operation. Due to the discrete nature of the fixed charges and trapped carriers, reliability problems in contemporary CMOS devices have a statistical nature [7].

For a particular average trapped charge density, the actual number of trapped charges vary from transistor to transistor, and their actual position in each transistor is unique. The impact of a particular trapped charge distribution on transistor characteristics is affected by the presence of other variability sources. Random discrete dopants, for example, result in current percolation around the dopants. The trapping of carriers in the vicinity of a dominant current percolation path can result in a dramatic change in the current or the threshold voltage.

For this reason, the starting point for the simulation of statistical reliability should be the simulation of the devices including all sources of variability that are appropriate for that device architecture. Random trapped charges can then be introduced to the original ensemble of these ‘fresh’ microscopically different transistors, and the corresponding change in the parameters can be recorded.

You can use the `reliability` command along with a number of options to add discrete trapped charges to the simulation domain as follows (see [reliability Command on page 882](#)):

```
reliability <option> <parameter>=<value>
```

---

## Interface-Trapped Charges

The `reliability ITC` command allows you to add interface-trapped charges (ITC) to each 'fresh' device in the ensemble with a given average sheet density that should be chosen to correspond to the required level of degradation. This sheet density is specified using the `density` parameter.

Traps are generated at the interface between an insulator and a semiconductor. In order to be general, you must specify the insulator material at whose interface the traps should be generated.

To restrict the presence of traps to a specific region or interface, you can specify a bounding box within which the traps can be added. By default, the bounding box is the entire device structure. It is not necessary to specify all bounds, as the maximum extent of the simulation domain in a given direction is used automatically if this boundary is not specified. Traps are generated at any interface between the specified insulator and any semiconductor, but only at points that lie within the bounding box.

For descriptions of the parameters specific to ITC, see [Generating Positions of Interface-Trapped Charges on page 883](#).

The following example generates traps statistically at the interface between silicon dioxide and a semiconductor material with a sheet density of  $1\text{e}12 \text{ cm}^{-2}$  but only between  $x=-15 \text{ nm}$  and  $x=+15 \text{ nm}$ :

```
reliability ITC status=on density=1e12 material=Oxide xmin=-15 xmax=15
```

**Note:**

Multiple `reliability ITC` commands are allowed to specify multiple insulator materials or different bounding regions. Therefore, it is required that all parameters for a particular trap region be specified on the one line.

---

## User-Specified Fixed Charge

In addition to automatically generating discrete fixed charges based on the nominal doping profile (RDD) or an interface sheet charge density (ITC), you can explicitly specify the location of discrete acceptor-type (negative) or donor-type (positive) charges. These charges can be added to the simulation structure by using the `reliability add` command:

```
reliability add charge=<string> x=<float> y=<float> z=<float>
```

The `charge` can be either `acceptor` or `donor`, or a fixed amount of charge (positive or negative) in units of the electronic charge as required, which is followed by the position in the 3D structure at which the charge should be placed (in the specified input units; default is nm).

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### Internal Sweep of Mobility Parameters

For descriptions of the relevant parameters, see [reliability Command on page 882](#).

The following command adds an acceptor-type charge at the (10.0, 5.0, 0.0) point in the structure:

```
reliability add charge=acceptor x=10.0 y=5.0 z=0.0
```

The following command applies a fixed amount of positive charge with magnitude  $2.5q$  (where  $q$  is the electronic charge in coulombs) at the (-40.0, 25.0, -10.0) point in the structure:

```
reliability add charge=+2.5 x=-40.0 y=25.0 z=-10.0
```

**Note:**

Multiple `reliability add` commands are allowed to include as many charges as required.

---

## Internal Sweep of Mobility Parameters

To facilitate, and potentially speed up, the calibration of Garand in TCAD to SPICE variability flows, you can run an internal sweep over specified mobility model parameters. For given bias conditions, Garand will sweep the mobility parameters over a list of values, calculating the device current for each parameter value. By only requiring one setup of the simulation structure, and reuse of previous solutions when mobility parameters change, the turnaround time for the calibration simulations can be reduced significantly.

To activate this feature, you specify the mobility parameter to be modified in a sweep (with full context) and a list of values over which you want to sweep, by using the `simulation mobility_sweep` command. The syntax is:

```
simulation mobility_sweep parameter=<string> values=<list>
```

where `parameter` specifies the full hierarchical material mobility parameter, and `values` specifies a comma-separated list of values over which the parameter is swept (see [Internal Sweep of Mobility Parameters on page 897](#)). For example:

```
simulation mobility_sweep \
    parameter=Silicon.conduction.mobility.strainx \
    values=1.0,1.25,1.5,1.75,2.0
simulation mobility_sweep parameter=Channel.conduction.caughey.vsat \
    values=1e7,5e7,1e8
```

As with specifying material parameters, you can change the mobility parameter for a material as a whole (`Silicon` in the example) or solely in a specific region (`Channel` in the example).

## Handling Multiple Mobility Sweeps

If you specify more than one `simulation mobility_sweep` command in a Garand input file, then you can choose how to interpret these commands by setting the mobility sweep mode.

### Grid Mode

In grid mode, multiple `simulation mobility_sweep` commands are taken to define a multidimensional grid in the mobility parameter space. In this case, every combination of the different parameter values will be simulated. For example, in the previous example that specified five values for `strainx` and three values for `vsat`, a total of 15 simulations will be run for each bias point, using every combination of the parameter values in the two lists.

To activate the grid mode, specify the following command:

```
simulation mobility_sweep_mode = grid
```

This is the default mode when multiple `simulation mobility_sweep` commands are given.

### Points Mode

In points mode, the values provided in `simulation mobility_sweep` commands are taken to define individual points in the mobility parameter space. If you specify  $n$  parameter values, then Garand will simulate  $n$  points in the sweep. For the  $i$ th simulation, Garand will use the  $i$ th value of each parameter in its list. This means that every `simulation mobility_sweep` command must specify the same number of values.

To activate the points mode, specify the following command:

```
simulation mobility_sweep_mode = points
```

---

## Specifying a Target Current

When performing a calibration, you want to find the value of the mobility parameter that will result in a current that matches the current in the target data against which you are calibrating. When running a mobility sweep, you can specify the target current that you are trying to obtain. Garand performs the sweep until it finds the two mobility parameter values that give currents that bound the target value, at which point, it will stop the sweep. This prevents running more simulations than are required to find the parameter values you are looking for.

To specify the target current, in A, for the mobility sweep, use the command:

```
simulation mobility_sweep_target=<float>
```

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### Additional Models

A target current can be specified if only one mobility parameter is being swept over multiple values. Additional `simulation mobility_sweep` commands can be present in the input file, but they must have only one value specified.

---

## Additional Models

This section discusses additional models.

---

### Density-Gradient Quantum Corrections

Although detailed quantum-mechanical simulators are available based on non-equilibrium Green's functions (NEGFs) [8][9] or the direct solutions of the Schrödinger equation [10], they are still computationally expensive. Computationally efficient methods to include the most important (first-order) quantum-mechanical effects are required for the purpose of practical computer-aided design of future generations of devices, especially when the important aspects of intrinsic parameter variability are concerned [11]. Therefore, the computational efficiency of the simulators used is essential.

First-order quantum corrections are usually introduced by an *effective quantum potential*. In this approach, the electrostatic potential used in classical simulators is modified by a 'quantum correction' term to mimic the required quantum-mechanical effects, thereby minimizing the change to the device simulators and maintaining the computational efficiency of preexisting simulators.

Although several different approaches have been proposed for including quantum corrections in classical and semiclassical simulations, the most popular is the density gradient (DG) approach and this method has been implemented in Garand.

The DG formalism introduces an additional quantum-correction term,  $\psi_{qm}$ , which is proportional to the second derivative of the square root of the carrier density:

$$\psi_{qm} = 2b_n \frac{\nabla^2 \sqrt{n}}{\sqrt{n}} = \phi_n - \psi + \frac{k_B T}{q} \ln\left(\frac{n}{n_i}\right) \quad (3)$$

where  $b_n = \hbar^2 / 12qm_n$ , and all other symbols have their usual meaning.

The DG equation can be calibrated against fully quantum-mechanical simulations based on a Poisson–Schrödinger solution or NEGF approach by considering the effective mass as a fitting parameter. In addition, the DG effective mass is considered to be anisotropic, so there are different effective mass components in each of the component directions,  $m_x$ ,  $m_y$ , and  $m_z$ .

## Chapter 3: Simulation Setup

### Additional Models

Therefore, the form of the DG equation solved is:

$$\frac{2b_n}{S} \left( \frac{1}{m_x} \frac{\partial^2 S}{\partial x^2} + \frac{1}{m_y} \frac{\partial^2 S}{\partial y^2} + \frac{1}{m_z} \frac{\partial^2 S}{\partial z^2} \right) = \phi_n - \psi + \frac{k_B T}{q} \ln \left( \frac{S^2}{n_i} \right) \quad (4)$$

where  $b_n = \hbar^2 / 12q$  and you solve for  $S = \sqrt{n}$ .

In other quantum-mechanical transport approaches such as NEGF, Neumann boundary conditions (NBC) are used in the source and drain, as the potential adjusts the electron injection to preserve charge neutrality. Garand implements such NBC [12], rather than Dirichlet boundary conditions for the potential at the Ohmic source/drain contacts as typically used in drift-diffusion simulations. NBC work better in conjunction with the DG in the sense that they do not restrict the potential and electron concentration in the source and drain from following the distribution imposed by quantum mechanics. This is particularly important in thin-body devices such as FinFETs and nanowires.

Ideally within DG simulations, values of the DG effective masses would be chosen to match the results obtained from fully quantum-mechanical simulations such as Poisson–Schrödinger or NEGF. The DG effective masses are material parameters. Therefore, if you want to change the default values to calibrate the quantum-mechanical corrections, use the `material` command in the input file.

For example, to change the DG effective masses for the conduction band in silicon, specify:

```
material Silicon.conduction.dgx 0.5
material Silicon.conduction.dgy 0.2
material Silicon.conduction.dgz 0.2
```

For example, to adjust the oxide masses, specify:

```
material Oxide.conduction.dgx 0.15
material Oxide.conduction.dgy 0.15
material Oxide.conduction.dgz 0.15
```

In the simulation of PMOS devices, the DG effective masses for the valence band are used. You activate DG quantum corrections by using the `model` command (see [Specifying Simple Models on page 859](#)).

## Boundary Conditions at Oxide Interfaces

The semiconductor–oxide boundary conditions for the quantum potential in the DG approach require careful consideration, and Garand uses the approach of Jin *et al.* [13]. This method fixes the gradient of the electron concentration perpendicular to the semiconductor–oxide interface depending in the relative effective masses in the semiconductor and the oxide, accounting for penetration of the electron wavefunction into the oxide.

## Chapter 3: Simulation Setup

### Additional Models

The electron density penetration as a function of distance,  $x$ , from the semiconductor–oxide interface can be approximated as:

$$n(x) = n(0)\exp\left(-\frac{2x}{x_p}\right) \quad (5)$$

where:

- $n(0)$  is the electron density at the interface.

- $x_p = -\frac{\hbar}{\sqrt{2m_{ox}\Phi_B}}$ .

This is the characteristic penetration depth obtained from the Wentzel–Kramers–Brillouin (WKB) approximation. Here,  $m_{ox}$  is the electron effective mass within the oxide and  $\Phi_B$  is the potential barrier of the oxide.

Using [Equation 5](#), the component of  $b_n \nabla \sqrt{n}$  normal to the semiconductor–oxide interface can be written as:

$$\mathbf{n} \cdot b_n \nabla \sqrt{n} = -\left(\frac{b_{ox}}{x_p}\right) \sqrt{n} \quad (6)$$

where  $b_{ox} = \frac{\hbar^2}{12qm_{ox}}$ .

The default oxide interface boundary conditions in Sentaurus Device do not modify the gradient of the carrier density in the same way as Garand does. This can present problems when trying to calibrate the effective mass parameters in Garand to match the carrier distribution in Sentaurus Device.

To apply Sentaurus Device boundary conditions in Garand, specify:

```
model dg_sdevice_bc = on
```

See [Specifying Simple Models on page 859](#).

Conversely, to activate the standard Garand boundary conditions in Sentaurus Device, include the following specification in the `Physics` section of the Sentaurus Device command file:

- `eQuantumPotential(AutoOrientation Density Formula=1)` for electrons
- `hQuantumPotential(AutoOrientation Density Formula=1)` for holes

## Other Density-Gradient Model Options

The effect of the boundary conditions at the semiconductor–oxide interface is to reduce the carrier concentration at the interface. This leaves uncompensated dopant atoms, which

## Chapter 3: Simulation Setup

### Additional Models

result in a spike in the electrostatic potential at the interface. This is expected behavior but, in highly doped source and drain regions, this uncompensated charge can be high. If it is not well resolved with a fine mesh, then the resultant spike in potential can be unphysically high. For this reason, you can limit the application of interface boundary conditions so that they are not applied if the source-type or drain-type doping concentration is higher than a specified value.

By default, this limit is set to  $1\text{e}20 \text{ cm}^{-3}$ , which can be modified with the following command:

```
model dg_doping_limit=<float>
```

where `dg_doping_limit` is the doping concentration in  $\text{cm}^{-3}$  (see [Specifying Simple Models on page 859](#)).

The following example prevents interface boundary conditions from being applied at interface mesh nodes where the doping concentration is greater than  $5\text{e}19 \text{ cm}^{-3}$ :

```
model dg_doping_limit = 5e19
```

When solving the density gradient equation for minority carriers, you can observe a similar effect at oxide interfaces with high minority-type doping. To avoid this, you can deactivate oxide interface boundary conditions for minority carriers with the command:

```
model minority_dg_bc = off
```

By default, the density gradient equation is solved in polysilicon gates. The main effect of this is to alter the depletion region at the polysilicon–gate oxide interface.

You can deactivate the solution within the polysilicon gate with the command:

```
model poly_dg = off
```

The DG quantum corrections provide another benefit. When simulating devices with random dopants, the sharp spikes in electrostatic potential created by each discrete dopant can trap carriers: electrons are trapped by donor ions and holes are trapped by acceptor ions.

Trapping majority carriers artificially reduces the conductivity of the device, resulting in a reduction in current, while trapping minority carriers in the bulk affects the depletion region. These effects are also mesh-spacing dependent. The inclusion of the DG solution in the simulation can minimize these effects [\[14\]\[15\]](#).

---

## Schrödinger Quantum Corrections

While DG quantum corrections efficiently capture first-order quantum-mechanical (QM) effects in the Garand simulator, a more advanced QM model is available in Garand that better captures the impact of physical confinement through self-consistent solution of the Poisson–Schrödinger equations. With the inclusion of a more advanced physical model, there is a compromise on the computational efficiency and care should be taken when using Poisson–Schrödinger QM models.

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If you specified `use_schrod_qc=on` (see [Simulation Setup on page 43](#)), then the QM charge density from the solution of the Schrödinger equation is used to obtain a ‘quantum correction’ term in the same way as for DG quantum corrections. Using the Schrödinger ‘quantum correction,’ the Garand drift-diffusion loop is performed in the same way as with DG quantum corrections (see [Modified Gummel Decoupled Method on page 160](#)) but with the Schrödinger solution being calculated rather than the solution of the DG equation. This Schrödinger solution is then used to calculate the quantum-corrected potential that is used in the solution of the current continuity equation.

If `use_schrod_qc` is not activated, the Poisson–Schrödinger model is coupled with the Garand drift-diffusion solution in stages to allow a more computationally efficient way of combining the impact of quantum confinement and carrier transport. To achieve this, the drift-diffusion simulation is performed until convergence, then the quasi-Fermi level from the converged drift-diffusion solution is used as a fixed reference within the Poisson–Schrödinger model to transfer the current transport behavior. The Poisson–Schrödinger model is then solved until convergence to obtain a QM solution of the charge density. This method is valid at low applied drain biases, including when an autoslice operation is used. [Figure 23 on page 127](#) outlines this simulation flow.

The following Schrödinger equation is solved with a spatially varying tensor effective mass, using the LAPACK libraries numerical eigenvalue problem solver [16]:

$$-\frac{\hbar^2}{2} \nabla \frac{1}{m_{ij}} \nabla \psi = (\psi - E) \psi \quad (7)$$

Dirichlet boundary conditions are applied, by default, to the outer bounds of the Schrödinger domain so that the wavefunction is zero. These boundary conditions are also applied within metals to ensure no penetration of the wavefunction into metallic regions. You can use the `enable_dirichlet_boundary` parameter to modify this default behavior (see [Poisson–Schrödinger Quantum Corrections on page 860](#)).

To solve the Schrödinger equation, the device is split into cross sections in the plane perpendicular to the direction of transport. Within each cross section, the Schrödinger equation is solved for each valley in the band structure independently, and the resultant charge density for a given cross section is taken as the sum of all valleys. Each cross section is then combined to reform the 3D solution of the charge density of the device. This 3D charge density is then used in the Poisson solver to obtain the updated potential.

Due to the nature of the Schrödinger solver, it can be computationally expensive in terms of both memory usage and CPU time required. The best way to reduce the computational overhead of your solution is to reduce the number of valleys included in the relevant material band structures, for example, by removing the unoccupied higher conduction valleys,  $L$  and  $\Gamma$ , from silicon. This can be achieved by removing the necessary valleys from the material definition (see [Removing a Valley Model on page 292](#)).

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### Additional Models

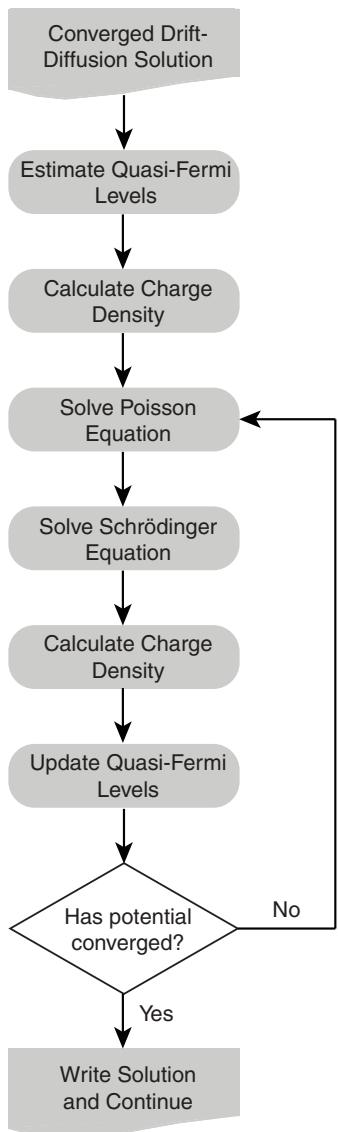
#### Note:

Energy subbands obtained from the solution of the Schrödinger eigenvalue problem are plotted in a specified output file as a function of the spatial coordinate along the transport direction. These are located within the output directory for each specific bias point.

You activate Poisson–Schrödinger quantum corrections by using the `model` command (see [Poisson–Schrödinger Quantum Corrections on page 860](#)):

```
model schrodinger <parameter>=<value>
```

*Figure 23 Flow diagram of the Poisson–Schrödinger model*



## Chapter 3: Simulation Setup

### Additional Models

## Defining 2D Confinement Directions

By default, the 2D Poisson–Schrödinger solver is selected (applies to FinFET or nanowire structures) and the confinement mass used in [Equation 7 on page 126](#) is extracted from the underlying band-structure model (ellipsoidal, multivalley for electrons, and six-band  $k\cdot p$  for holes) including the effects of applied stress and can be checked in the material model file written into the results directory.

Confinement directions can be defined for the relevant semiconductor materials. For example, if the channel is along the x-direction, then for a silicon-based device, the confinement would be defined as:

```
material Silicon.x_confinement off
material Silicon.y_confinement on
material Silicon.z_confinement on
```

This is combined with the definition of the orientation. For example:

```
material Silicon.crystal.x 1 1 0
material Silicon.crystal.z 0 0 1
```

This would align the channel along the [110] direction with a sidewall orientation of (110) and a substrate on (001).

You can overwrite the default confinement masses by using the input file with the following commands:

```
material Silicon.conduction.X1.mqy 0.3
material Silicon.conduction.X2.mqy 0.3
material Silicon.conduction.X3.mqy 0.3
material Silicon.conduction.X4.mqy 0.3
material Silicon.conduction.X5.mqy 0.3
material Silicon.conduction.X6.mqy 0.3
material Silicon.conduction.X1.mqz 0.6
material Silicon.conduction.X2.mqz 0.6
material Silicon.conduction.X3.mqz 0.6
material Silicon.conduction.X4.mqz 0.6
material Silicon.conduction.X5.mqz 0.6
material Silicon.conduction.X6.mqz 0.6
```

These commands set the confinement masses in the delta valleys of silicon to 0.3 in the y-direction (sidewall) and 0.6 in the z-direction. It is necessary to specify values for all equivalent valleys (X1, X2, X3, X4, X5, and X6); otherwise, default values apply. Similar syntax can be used for the hole masses:

```
material Silicon.valence.HH.mqy 0.3
material Silicon.valence.HH.mqz 0.6
```

## Defining 1D Confinement

For simulation of structures with 1D confinement (bulk or FDSOI architectures for example), set the following parameters:

```
model schrodinger confinement=1D
model schrodinger 1d_confinement_direction=z
```

See [Poisson–Schrödinger Quantum Corrections on page 860](#).

Using the same orientation as for the 2D example, this would result in confinement normal to the (001) surface.

The confinement directions can then be identified as:

```
material Silicon.x_confinement off
material Silicon.y_confinement off
material Silicon.z_confinement on
```

The same syntax can be used for the redefinition of the confinement masses, although only the masses for the z-direction need be considered.

## Adding Schrödinger Boundaries

In certain FET structures such as FinFET devices, there might not be a well-defined energy barrier around the area of interest. The fin is the active area of interest regarding 2D confinement.

However, the bottom of the fin might not have an energy barrier, such as those found at oxide interfaces, leading to an open Schrödinger boundary condition in this region.

Although the Schrödinger solver enforces a Dirichlet boundary condition by default (which you can deactivate by setting `enable_dirichlet_boundary=off`), such that the wavefunction is zero at the outer bounds of the Schrödinger domain, it is sometimes preferable to also enforce an energy barrier to obtain a better defined solution. You can define a region in the device where an artificial energy barrier, or boundary, can be specified.

In cases where there is an open boundary condition for the Schrödinger equation, set `enable_complex_checks=on`, which will inform you whether any of the used solutions are complex. If possible, avoid complex solutions by applying appropriate boundary conditions. See [Poisson–Schrödinger Quantum Corrections on page 860](#).

To add an energy barrier in the simulation domain, use the following syntax:

```
model schrodinger boundary <parameter>=<value>
```

For the parameters specific to Schrödinger boundaries, see [Schrödinger Boundary Conditions on page 862](#).

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### Additional Models

## Quantum-Confining Valley Splitting or Separation

The intervalley energy separation is altered in a quantum-confined system as the energy of the lowest-lying subband of a given valley represents the valley energy minimum. This lowest-lying subband depends on the confinement applied and the effective mass in the confinement direction. Therefore, lighter effective-mass valleys will be pushed higher in energy than heavier effective-mass valleys. This change in the valley minimum can cause valley splitting, or a reduction in intervalley energies, which in turn affects carrier transport.

When you activate both the Poisson–Schrödinger model and Monte Carlo transfer (MCT) file output (see [Monte Carlo Transfer Files on page 48](#)), the simulation automatically calculates the intervalley energy separation as modified by any quantum confinement. The intervalley energy separations are written to a `.pst` file alongside the MCT file and is used to modify the Monte Carlo simulation.

---

## Fermi–Dirac Carrier Statistics

The basic drift-diffusion simulation model is developed around the use of Maxwell–Boltzmann carrier statistics, which are an approximation of Fermi–Dirac carrier statistics. Maxwell–Boltzmann statistics are valid for semiconductors that are in a nondegenerate condition, where only the tail of the carrier distribution function is important.

The nondegenerate condition tends to be the case for most semiconductors at or above room temperature at low doping and charge densities. In particular, the silicon semiconductor material is a case where degenerate conditions do not play a strong role in the transport. There are some semiconductor materials, such as the III–V semiconductor InGaAs, where degenerate conditions play a very strong role and must always be considered.

A general rule for assessing whether degeneracy plays a role in a semiconductor material is whether the effective density-of-states (DOS), often referred to as  $N_C$  for the conduction band and  $N_V$  for the valence band, is smaller than the typical charge densities apparent in the FET simulation. If it is smaller, then degenerate conditions occur and Fermi–Dirac carrier statistics must be activated.

### Note:

Take care when activating Fermi–Dirac carrier statistics because they introduce some additional computational overhead and might cause convergence instability relating to mesh density (Fermi–Dirac carrier statistics might require finer meshing for stable solutions).

In Garand, Fermi–Dirac carrier statistics are applied consistently and coherently within each component of the simulation. This results in modifications to the Poisson solver, the density gradient solver, the Schrödinger solver, and the current continuity solver. Fermi–Dirac

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carrier statistics are applied within a multivalley model that includes nonparabolicity corrections and are computed for both majority and minority carriers in any given simulation.

The electron and hole concentrations in this case can be written as:

$$\begin{aligned} n &= N_C F_{1/2}(\eta_n) \\ p &= N_V F_{1/2}(\eta_p) \end{aligned} \quad (8)$$

where  $\eta_i = \frac{E_{f,i} - E_c}{k_B T}$  and  $F_{1/2}$  is the Fermi integral of order one-half.

In the drift-diffusion framework, it is straightforward to demonstrate that the current continuity equation can be still written in a Boltzmann-like form provided that the Einstein diffusion relation is modified from:

$$D = \frac{k_B T}{q} \mu \quad (9)$$

to:

$$D = \frac{F_{1/2}(\eta)}{F_{-1/2}(\eta)} \frac{k_B T}{q} \mu \quad (10)$$

and  $F_{-1/2}$  is the Fermi integral of order  $-1/2$ .

You can also easily demonstrate that this approach is equivalent to keeping the conventional Einstein diffusion relation, but rewriting the current density from:

$$\vec{f} = \mu (\vec{q}n\vec{E} + k_B T \nabla n) \quad (11)$$

to:

$$\vec{f} = \mu (\vec{q}n\vec{E} + k_B T \nabla n - nk_B T \nabla (\ln(\gamma))) \quad (12)$$

where  $\gamma = \frac{F_{1/2}(\eta)}{\exp(\eta)}$ .

Therefore, when Fermi–Dirac statistics are adopted, the formulas of the drift-diffusion approach remain valid provided an extra term in the carrier driving-force is introduced or, alternatively, a modified non-Einstein mobility-diffusion relation is adopted.

To activate Fermi–Dirac statistics, use the `model` command (see [Fermi–Dirac Statistics on page 863](#)):

```
model fermi_dirac <parameter>=<value>
```

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The formal mathematical definition of the Fermi–Dirac integrals applied in the carrier statistic equations is:

$$\frac{n}{N_C} = \sum_i \frac{Z_i m_{d,i}^*}{Z_{\min} m_{d,\min}^*} \left( F_{1/2}(\eta - \eta_i) + \frac{15}{4} \alpha_i k_B T F_{3/2}(\eta - \eta_i) \right) \quad (13)$$

where:

- $i$  denotes the valley index.
- $Z_i$  is the degeneracy of valley  $i$ .
- $m_{d,i}^*$  is the density-of-states mass of valley  $i$ .
- $\alpha_i$  is the nonparabolicity parameter of valley  $i$ .
- The Fermi–Dirac integral of order  $j$  is  $F_j = \frac{1}{\Gamma_{j+1}} \int_0^\infty \frac{x^j}{1 + \exp(x - \eta)} dx$ .
- The intervalley separation between valley  $i$  and the minimum valley of the band is  $\eta_i = \frac{E_i - E_{\min}}{k_B T}$ .

---

## Contact Resistance

You can apply a contact resistance to the source and drain contacts. This resistance can be specified either as a single lumped resistor with a given resistance in ohms [ $\Omega$ ] or as a contact resistivity in  $\Omega \cdot \text{cm}^2$  that can either be applied as a lumped resistance or be distributed across the area of the contact.

## Specifying a Lumped Contact Resistance

To specify a lumped contact resistance, use the following command (see [contact Command on page 849](#)):

```
contact resistance_lumped=<float>
```

The specified value is the contact resistance in ohms [ $\Omega$ ] that will be applied to both contacts. The potential on the source and drain contacts will be uniformly modified to account for the voltage drop across the lumped resistance leading to a reduced effective applied drain voltage, that is,  $V_{\text{Deff}} = V_d - 2RI_d$ .

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### Additional Models

You can also set the source and drain contact resistances independently, as follows:

```
contact resistance_lumped_source=<float>
contact resistance_lumped_drain=<float>
```

During the Gummel iterations, the source and drain contact potentials can be updated at the start of the iteration to reflect the voltage drop across the external contact resistances. This is not done at every iteration to allow the solution to stabilize before the contact potentials are updated.

The application of the contact potential update is determined by the relative difference in current from one iteration to the next:

- If the relative difference is greater than  $10^{-1}$ , then the contact potential is *not* updated.
- If the relative difference is less than  $10^{-1}$ , then the contact potential is updated.

You can adjust this upper threshold by setting the following command:

```
contact resistance_convergence_max=<float>
```

There is also a lower threshold (by default  $5 \times 10^{-4}$ ) below which the contact potential is also not updated. This allows for a stable final convergence in a regime where further changes to the contact potential would have little effect on the calculated current. You can adjust this lower threshold by setting the following command:

```
contact resistance_convergence_min=<float>
```

In addition, to help overall convergence, the update to the contact potential is damped by a damping factor `resistance_damping` (0.25 by default), which can be adjusted by using the command:

```
contact resistance_damping=<float>
```

#### Note:

A distributed contact resistance is not an option when specifying a value of contact resistance in ohms.

## Specifying Resistivity

This section describes how to specify different types of resistivity.

### Lumped Resistivity

The specified value is the contact resistivity ( $\rho_c$ ) in  $\Omega \cdot \text{cm}^2$  that will be applied to both contacts. The equivalent lumped resistance is obtained from the integration of the conductivity ( $1/\rho_c$ ) over each node in the contact. The potential on the source and drain contacts will be uniformly modified to account for the voltage drop across the lumped resistance leading to a reduced effective applied drain voltage, that is,  $V_{\text{Deff}} = V_d - 2RI_d$ .

## Chapter 3: Simulation Setup

### Additional Models

You can also set the source and drain contact resistivities independently, as follows:

```
contact resistivity_lumped_source=<float>
contact resistivity_lumped_drain=<float>
```

Lumped resistance specified by a resistivity is applied in the same way as lumped resistance described in [Specifying a Lumped Contact Resistance on page 132](#). The same options for `resistance_convergence_min` and `resistance_damping` are also available in this case.

### Distributed Resistivity

To specify distributed resistivity, use the following command:

```
contact resistivity_distrib=<float>
```

The specified value is the contact resistivity ( $\rho_c$ ) in  $\Omega \cdot \text{cm}^2$  that will be applied to both contacts. This resistivity is used to calculate the contact resistance of each mesh node on the contact based on the contact area associated with that node. The boundary conditions for the current continuity equation at the source/drain contacts are modified to be consistent with the current flow into or out of each node through the resistance at that point.

You can also set the source and drain contact resistivities independently:

```
contact resistivity_distrib_source=<float>
contact resistivity_distrib_drain=<float>
```

#### Note:

Solving with distributed contact resistance is slower than with lumped resistance. The difference in current obtained with the two methods is usually small. Therefore, use lumped resistance unless there is a demonstrable difference in current between the two methods.

---

## Drain Leakage

You switch on a drain leakage simulation and select the model to use for the leakage calculation by specifying the following command (see [Band-to-Band Tunneling Model on page 864](#)):

```
model drain_leakage status=on method=<string>
```

The `method` parameter sets the model to use for the leakage calculation:

- `local` selects the local band-to-band model (see [Modified Kane Local Model](#)).
- `nonlocal` selects the nonlocal band-to-band model (see [Dynamically Adapted Nonlocal Model on page 137](#)).

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### Additional Models

## Modified Kane Local Model

You can simulate drain leakage by using a local band-to-band electron–hole pairs generation model, which is based on the original work of Kane [17]. You can calculate the generation rate  $G$  [ $\text{cm}^{-3} \text{s}^{-1}$ ] for both direct and indirect transitions in the band gap according to the following relation [18]:

$$G = G_{\text{dir}} + G_{\text{indir}} \quad (14)$$

where the direct and indirect components are:

$$\begin{aligned} G_{\text{dir}} &= A_{\text{dir}} \left( \frac{F}{F_0} \right)^{P_{\text{dir}}} \exp \left( -\frac{B_{\text{dir}}}{F} \right) \\ G_{\text{indir}} &= A_{\text{indir}} \left( \frac{F}{F_0} \right)^{P_{\text{indir}}} \exp \left( -\frac{B_{\text{indir}}}{F} \right) \end{aligned} \quad (15)$$

with the direct tunneling Kane coefficients expressed by:

$$\begin{aligned} A_{\text{dir}} &= \left( \frac{9}{\pi^2} \right) \frac{g \pi \sqrt{m_r} (qF_0)^{P_{\text{dir}}}}{9h^2 \sqrt{E_g^\Gamma}} \\ B_{\text{dir}} &= \frac{\pi^2 \sqrt{m_r (E_g^\Gamma)^3}}{qh} \end{aligned} \quad (16)$$

and the indirect tunneling Kane coefficients expressed by:

$$\begin{aligned} A_{\text{indir}} &= \frac{9 \sqrt{(m_c m_v)^3} (1 + 2N_{\text{ph}}) D_{\text{ph}}^2 (qF_0)^{P_{\text{indir}}}}{2^{21/4} h^{5/2} m_r^{5/4} \rho \epsilon_{\text{ph}} E_g^{7/4}} \\ B_{\text{indir}} &= \frac{2^{7/2} \pi \sqrt{m_r (E_g)^3}}{3qh} \end{aligned} \quad (17)$$

where:

- $F$  is the local electric field.
- $F_0$  is a normalization field (1 V/cm).
- $P_{\text{dir}} = 2.0$  for direct tunneling.
- $P_{\text{indir}} = 2.5$  for indirect tunneling.
- $g$  is a degeneracy factor.
- $m_r$  is the reduced tunneling mass.
- $q$  is the elementary charge.
- $h$  is Planck's constant.
- $E_g^\Gamma$  is the direct band gap at the  $\Gamma$ -point.

## Chapter 3: Simulation Setup

### Additional Models

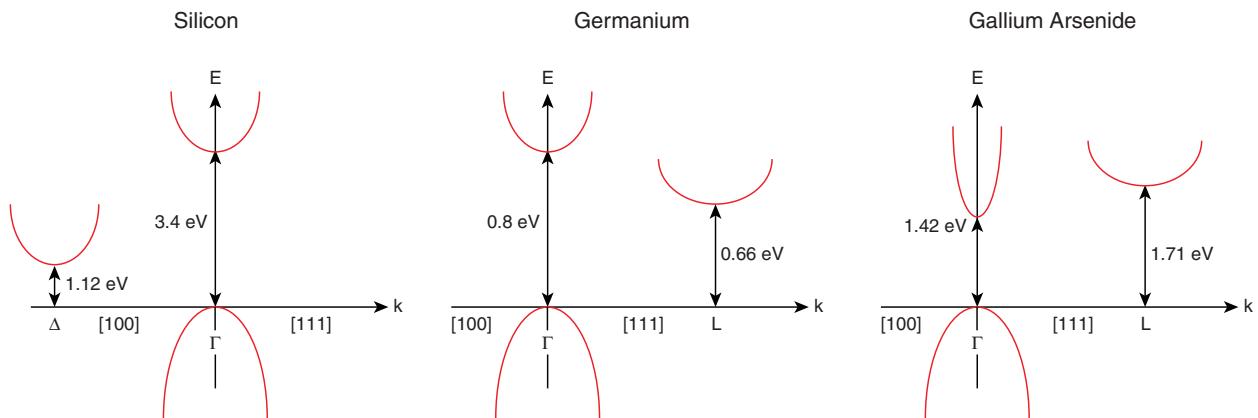
- $m_v$  ( $m_c$ ) is the valence (conduction) band density-of-states effective mass.
- $N_{ph} = 1/[\exp(\epsilon_{ph}/kT) - 1]$  is the Bose function for the phonons at temperature  $T$ , with  $k$  being the Boltzmann constant.
- $D_{ph}$  is the deformation potential associated with the selected phonons.
- $\rho$  is the mass density.
- $\epsilon_{ph}$  is the phonon energy.
- $E_g$  is the minimum band gap.

In Garand, these coefficients are calculated directly using the material parameters supplied by the material database. You can also specify the  $A$ ,  $B$ , and  $P$  parameters directly in the input file, which might be more convenient when trying to fit experimental leakage data. If these values are specified, then only one component (that is, one of 3.20 and 3.21) is applied using the provided values. You must select  $P$  to reflect whether the material has a direct ( $P = 2.0$ ) or indirect ( $P = 2.5$ ) band gap.

It should be noted that, for materials exhibiting an electronic band gap much smaller than  $E_g$  (for example, silicon), the indirect band-to-band component will dominate the leakage. On the other hand, for materials having  $E_g$  comparable to the electronic band gap (for example, germanium), direct and indirect band-to-band components become equally important with one slightly dominating the other depending on the applied voltage conditions. Finally, for materials with a direct electronic band gap (for example, GaAs), the leakage will be ruled by the direct band-to-band transitions and the indirect component is neglected in Garand.

[Figure 24](#) is a schematic representation of band structures for silicon, germanium, and GaAs to help visualize the relative importance of direct and indirect transitions based on the magnitude of the  $\Gamma$ -point and the electronic gaps.

**Figure 24 Schematic band structure for (left) silicon, (middle) germanium, and (right) gallium arsenide**



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### Additional Models

To avoid artifacts in the band-to-band leakage introduced by electric field peaks at the semiconductor–dielectric interface (especially in the presence of density-gradient quantum corrections), you can specify in the input file a minimum distance (`min_dist`) from the interface from which to start to calculate the tunneling. In most cases, a distance of 1–2 nm is sufficient.

### Specifying Fraction of Band Gap

It is also well known that local models tend to overestimate the leakage current as the leakage is simply a function of the local electric field, and the calculation ignores the real band profiles and the occupation of states at the start and end tunneling points. In order for band-to-band tunneling to occur, there must be an overlap in energy between the valence and conduction bands within a short enough distance. Therefore, it is expected that there will be a change in the band edges approximately equal to the band gap of the material. In Garand, the parameter `deltapot` specifies a fraction of the band gap that must be used to determine whether tunneling at a point is included.

If the conduction band edge varies by more than  $\text{deltapot} \times qE_g/2$  in the direction of the electric field within a distance of  $\text{deltapot} \times qE_g/F$ , where  $F$  is the electric field magnitude, then tunneling at that node is included. This is particularly effective at removing tunneling from interface regions where there would be no states to tunnel from or to due to the oxide. This feature adds a degree of nonlocality to the local tunneling model and is activated by default with a value of `deltapot=1.0`. However, it can introduce some numeric instability and can be switched off by setting `deltapot=0.0`.

To switch on a drain leakage simulation that uses the local band-to-band tunneling model, use the command:

```
model drain_leakage status=on method=local <parameter>=<value>
```

For descriptions of the parameters, see [Band-to-Band Tunneling Model on page 864](#).

### Dynamically Adapted Nonlocal Model

To overcome the intrinsic limitations associated with an analytic local model (see [Modified Kane Local Model on page 135](#)), a full numeric calculation of the tunneling currents can be performed taking into account:

1. The realistic shape of the conduction and valence band

This goal is achieved by a numeric integration of the tunneling barrier under the WKB approximation [19].

2. The proper occupation of available states at the starting and arriving tunneling points

This goal is achieved by computing the Fermi–Dirac distributions at either end of the tunneling path.

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### Additional Models

Because most band-to-band leakage models available in the literature are one dimensional, the common approach adopted in TCAD simulation is to perform the tunneling calculation along several 1D paths chosen to lay along the direction of the maximum electric field.

The term *dynamically adapted* refers to the way these paths are determined at each simulation step accordingly to the up-to-date electrostatic configuration. For each of these paths, the conduction band and the valence band are interpolated on a fine 1D mesh, which is independent from the main simulation mesh.

The term *non/local* refers to the fact that the electrons are tunneling from a starting point in the valence band to a spatially separated arriving point in the conduction band. Therefore, the tunneling rate no longer depends solely on the local electric field at the starting point, but it depends on the full tunneling barrier profile and on the occupation of states at the two ends of the tunneling path.

For each mesh point, you can dynamically determine the 1D tunneling direction (here called  $x$  for convenience) and express the band-to-band generation as:

$$qG_e = -\frac{dJ_n}{dx} \quad (18)$$

Given that local mesh spacing  $dx$  and local energy spacing  $dE$  are related directly by the local electric field  $F$ , [Equation 18](#) can be rewritten as:

$$G_e = |F| \frac{dJ_n}{dE} \quad (19)$$

The tunneling current,  $J$ , can be expressed by the general Landauer approach:

$$J = \frac{2q}{2\pi h A} \int_{\mathbf{k}_\perp} T(E, \mathbf{k}_\perp) \{f_v(P_1) - f_c(P_2)\} dE \quad (20)$$

where:

- $A$  is a normalizing area.
- $f_v$  and  $f_c$  are the Fermi–Dirac functions at the start point (valence band) and end point (conduction band).
- $T$  is the tunneling probability and, under the WKB approximation, can be computed as:

$$T = \frac{\pi^2}{9} \exp(-2 \int \text{Im}(k_x) dx) \approx \frac{\pi^2}{9} \exp(-2 \int k dx) \exp\left(-|\mathbf{k}_\perp|^2 \int \frac{dx}{k}\right) \quad (21)$$

$$\text{using the approximation } \text{Im}(k_x) = \sqrt{k^2 + |\mathbf{k}_\perp|^2} \approx k + \frac{|\mathbf{k}_\perp|^2}{2k}.$$

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Considering that:

$$\frac{dJ}{dE} = \frac{q}{4\pi^3 \hbar} \int T(E, \mathbf{k}_\perp) d\mathbf{k}_\perp (f_v - f_c) \quad (22)$$

the band-to-band generation is finally expressed as:

$$G = \frac{g|\nabla E_v(P_1)|}{36\hbar} \left( \int_{P_1}^{P_2} \frac{dx}{k} \right)^{-1} \left\{ 1 - \exp \left( -k_{\max}^2 \int_{P_1}^{P_2} \frac{dx}{k} \right) \right\} \exp \left( -2 \int_{P_1}^{P_2} k dx \right) \{f_v(P_1) - f_c(P_2)\} \quad (23)$$

where  $k_{\max}$  is determined to conserve the perpendicular momentum by ensuring that the tunneling energy is limited between:

$$E_{c,\min} + \frac{\hbar^2 |\mathbf{k}_{\perp, \max}|^2}{2m_c} \leq E < E_{v,\max} - \frac{\hbar^2 |\mathbf{k}_{\perp, \max}|^2}{2m_v} \quad (24)$$

while the magnitude of the wavevector  $k$  is obtained by inverting the Kane two-band dispersion relation [19][20]:

$$E_\pm = \frac{E_G}{2} + \frac{\hbar^2 k^2}{2m_0} \pm \frac{1}{2} \sqrt{E_G^2 + \frac{E_G \hbar^2 k^2}{2m_r}} \quad (25)$$

The generation rate calculated by Equation 23 is strictly valid for direct bandgap semiconductors. For indirect bandgap semiconductors such as silicon, Equation 23 is modified slightly, according to the Vandenberghe approach [21]. In this case, the prefactor is modified to take into account the interaction with phonons by using the same parameters appearing in the Kane approach:

- $N_{ph}$  is the Bose function for the phonon population.
- $D_{ph}$  is the deformation potential.
- $\rho$  is the mass density.
- $\varepsilon_{ph}$  is the phonon energy.

Moreover, in this case, the  $E(k)$  dispersion in the band gap is simplified from the Kane (two-band) dispersion to two simpler effective mass dispersions for the valence and conduction bands separately. This is possible because the link between the two branches is now assured by the phonons.

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Therefore, the generation rate for phonon-assisted indirect tunneling is:

$$G = A_{\text{ph}} \left( \int_{P_1}^{P_0} \frac{dx}{k_v} \right)^{-1} \left( \int_{P_0}^{P_2} \frac{dx}{k_c} \right)^{-1} \left\{ 1 - \exp \left( -k_{v,\max}^2 \int_{P_1}^{P_0} \frac{dx}{k_v} \right) \right\} \left\{ 1 - \exp \left( -k_{c,\max}^2 \int_{P_0}^{P_2} \frac{dx}{k_c} \right) \right\} \\ \times \exp \left[ -2 \left( \int_{P_1}^{P_0} k_v dx + \int_{P_0}^{P_2} k_c dx \right) \right] \{f_v(P_1) - f_c(P_2)\} \quad (26)$$

where  $P_0$  is the coordinate in real space where  $k_c = k_v$ , and where the multiphonon prefactor is given by:

$$A_{\text{ph}} = \frac{g |\nabla E_v(P_1)| \sqrt{(m_c m_v)} (1 + 2N_{\text{ph}}) D_{\text{ph}}^2}{2^{19/4} \pi^2 h^{1/2} m_r^{1/4} \rho \epsilon_{\text{ph}} E_g^{3/4}} \quad (27)$$

Drain leakage simulation using the nonlocal band-to-band model can be activated using the command:

```
model drain_leakage status=on method=nonlocal
```

There are no additional parameters for the nonlocal model (see [Band-to-Band Tunneling Model on page 864](#)).

## Shockley–Read–Hall Generation–Recombination

Garand includes the Shockley–Read–Hall (SRH) model for generation–recombination due to defect levels within the energy gap. This can act as a source of leakage current in MOSFET devices. As Garand models transport of majority carriers only, local generation–recombination cannot be included self-consistently.

To include the effects of SRH, the calculated generation rate at each mesh point in the drain region is integrated to obtain the total majority charge generated per second. It is then assumed that all of the generated charge will flow to the drain contact and contribute to the total drain current. Likewise, it is assumed that the total integrated minority charge generated will contribute to the substrate current.

### Basic Shockley–Read–Hall

The SRH model is implemented with the following formula:

$$R_{\text{net}}^{\text{SRH}} = \frac{n p - n_{i,\text{eff}}^2}{\tau_p(n + n_1) + \tau_n(p + p_1)} \quad (28)$$

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where:

- $n_1 = n_{i,\text{eff}} \exp\left(\frac{E_{\text{trap}}}{kT}\right)$  and  $p_1 = n_{i,\text{eff}} \exp\left(\frac{-E_{\text{trap}}}{kT}\right)$ .
- $E_{\text{trap}}$  is the difference in energy, in eV, between the trap level and the intrinsic Fermi level, where positive values represent a trap level closer to the conduction band, and negative values are closer to the valence band.

As with other models in Garand, setting `status=on` for the SRH model activates the model for the simulation. For example:

```
model srh status=on <parameter>=<value>
```

For descriptions of the parameters, see [Shockley–Read–Hall Generation–Recombination on page 865](#).

If you set `doping_dependence=on`, then the lifetimes for electrons and holes will be modified to account for the total doping concentration at each mesh node, as described in [Doping Dependence](#).

## Doping Dependence

If you activate doping dependence for the SRH model, then the lifetimes used in the SRH equation are modified based on the acceptor and donor concentrations, using the following formula:

$$\tau_{\text{dop}}(N_{A,0} + N_{D,0}) = \tau_{\text{min}} + \frac{\tau_{\text{max}} - \tau_{\text{min}}}{1 + \left(\frac{N_{A,0} + N_{D,0}}{N_{\text{ref}}}\right)^\gamma} \quad (29)$$

where:

- $\tau_{\text{max}}$  is the lifetime parameter specified for the basic SRH model above.
- $\tau_{\text{min}} = 0$ .
- $N_{\text{ref}} = 1\text{e}16$ .
- $\gamma = 1$ .

---

## Trap-Assisted Tunneling

By including trap-assisted tunneling (TAT) in the SRH model, the generation rate will be enhanced due to a reduction in the lifetimes calculated from the following equation:

$$\tau = \frac{\tau_0}{1 + \Gamma_{\text{TAT}}} \quad (30)$$

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Here,  $\Gamma_{\text{TAT}}$  is the trap-assisted tunneling factor, which is primarily dependent on the electric field. Garand offers different methods to calculate  $\Gamma_{\text{TAT}}$ : a local model and a nonlocal model.

The input file command for including TAT in the SRH model is as follows:

```
model tat_leakage status=on <parameter>=<value>
```

For descriptions of the parameters, see [Trap-Assisted Tunneling for Shockley–Read–Hall Model on page 869](#).

The `method` parameter specifies whether to use the local or nonlocal TAT model.

**Note:**

The nonlocal model is used only to calculate the TAT factor for discrete traps (see [Discrete Traps on page 143](#)).

For the background SRH generation, the local model is always used to reduce the computational overhead, as this is calculated at every mesh point.

The `tunnel_mass_n` and `tunnel_mass_p` parameters set the tunneling mass for the electrons and holes, respectively, used in both the local and nonlocal TAT models.

## Local Trap-Assisted Tunneling Model

The local TAT model is implemented according to the Hurkx approximation [22]. In this case, the leakage enhancement due to TAT is defined as:

$$\Gamma_{n,p} = \frac{\Delta E_{n,p}}{kT} \int_0^1 \exp\left[\frac{\Delta E_{n,p}}{kT} u - K_{n,p} u^{3/2}\right] du \quad (31)$$

where:

- $K_{n,p} = \frac{4}{3} \frac{\sqrt{2m^* \Delta E_{n,p}^3}}{q\hbar|F|}$ .
- $\Delta E_n$  is the energy difference between the trap energy (given by  $E_{\text{trap}}$ ) and the conduction band edge.
- $\Delta E_p$  is the energy difference between the trap energy and the valence band edge.
- The quantity  $F$  is the local electric field at the trap position, which is numerically computed as the lowest between the field from the real electrostatic potential, the field from the quantum-corrected effective potential, and the `max_field` value (user-defined parameter; see [Trap-Assisted Tunneling for Shockley–Read–Hall Model on page 869](#)). This is to limit the overestimation of TAT due to both large mesh-dependent electric fields at the locations of discrete dopants and large quantum-corrected electric fields at oxide interfaces.

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## Nonlocal Trap-Assisted Tunneling Model

In the nonlocal case, the TAT enhancement factor is computed without using the Hurkx approximation, but by fully integrating the product of net flux (carrier density multiplied by the thermal velocity) and the tunneling probability for each energy between the trap level and the bottom of the conduction band (for electrons, a similar equation holds for holes with respect to the valence band) [22]:

$$\Gamma_n = \frac{1}{kT} \int \exp\left(\frac{E_c - E_x}{kT}\right) T(E_x) dE_x \quad (32)$$

where  $E_x$  is the energy to which the electron (or hole) is tunneling, and  $T(E_x)$  is the tunneling probability for that particular energy level. This probability is calculated numerically using a Wentzel–Kramers–Brillouin (WKB) integral over a densely interpolated 1D auxiliary mesh along the direction of the maximum field from the position of each discrete trap.

In the case of a perfectly triangular barrier (which is a valid approximation at very high electric fields), the Hurkx approximation is an excellent solution of the full flux integral, and both local and nonlocal models converge to the same results.

For the parameter specific to the nonlocal TAT model, see [Trap-Assisted Tunneling for Shockley–Read–Hall Model on page 869](#).

---

## Discrete Traps

Garand allows a list of discrete trap locations to be set up and the generated charge from each of these traps to be included within the overall generated SRH charge. Trap positions can be either specified explicitly in the Garand input file or generated randomly within a region of the device. The methods for generating trap positions are described here.

When dealing with leakage from discrete traps, a reformulated version of the equation for SRH generation is used. The lifetimes,  $\tau$ , are defined in terms of the trap density,  $N_0$ , and the trap cross-section,  $\sigma$ , as:

$$\tau = \frac{1}{N_0 \sigma v_{th}} \quad (33)$$

where the thermal velocity,  $v_{th}$ , is calculated as:

$$v_{th} = \sqrt{\frac{2k_B T}{m}} \quad (34)$$

in which  $m$  is the effective mass of the carrier being considered.

This allows the SRH formula to be rewritten as:

$$R_{net}^{SRH} = \frac{N_0 v_{th}^n v_{th}^p \sigma_n \sigma_p (np - n_{i,eff}^2)}{v_{th}^n \sigma_n (n + n_1) + v_{th}^p \sigma_p (p + p_1)} \quad (35)$$

## Chapter 3: Simulation Setup

### Additional Models

Rather than being applied at every point in the simulation mesh, the SRH generation from the discrete trap is calculated only at the eight corner nodes of the mesh element within which a trap is located. Using the same cloud-in-cell charge assignment method used for random discrete dopants, a fraction of the trap,  $X$ , is allocated to each corner node of the mesh element. The trap density that is used in [Equation 35](#) at each corner node,  $(i, j, k)$ , is then set as:

$$N_0(i, j, k) = \frac{X_{i, j, k}}{V_{i, j, k}} \quad (36)$$

where  $V_{i, j, k}$  is the volume associated with the mesh node at point  $(i, j, k)$  within the simulation mesh. In this way, integrating the total trap density over the mesh element results in exactly one, giving the effect of exactly one trap at the specified position.

The different methods to introduce traps allow the specification of the trap cross-section,  $\sigma_0$ , for electrons and holes. In this formulation of [Equation 35](#), TAT is applied as a modification to the trap cross-section as:

$$\sigma = \sigma_0(1 + \Gamma_{\text{TAT}}) \quad (37)$$

where  $\Gamma_{\text{TAT}}$  is calculated from either the local or nonlocal TAT model as previously described.

## User-Specified Trap Positions

The positions of discrete traps to include in the SRH generation calculation can be set explicitly in the Garand input file with the command:

```
model srh add_trap <parameter>=<value> <parameter>=<value> ...
```

For descriptions of the parameters, see [User-Specified Trap Positions on page 866](#).

The location of the trap is given with the  $x$ ,  $y$ , and  $z$  parameters. Coordinates are in nm unless the input units have been changed.

The energy level of each trap is set with the `trap_energy` parameter. If you do not set its value explicitly here, then the value used for the basic SRH model will also be used here.

The trap cross-sections for electrons (`xsec_n`) and holes (`xsec_p`) control the generation rate following [Equation 35](#).

Multiple `add_trap` commands can be used, depending on the number of traps to be included. Therefore, each command to add a trap must be on a single line in the input file. For example:

```
model srh add_trap x=25 y=0 z=-70 trap_energy=0.0 xsec_n=1e-15 \
xsec_p=1e-15
```

**Note:**

If the only discrete traps are those added using this method, then the contribution from the traps to the overall leakage current will be calculated at each Gummel iteration and included in the total leakage current calculated and output at that point.

## Random Trap Positions

To investigate statistical variability in leakage current due to generation from discrete traps, trap positions can be generated randomly within a specified region of the device. By default, the number of traps generated follows a Poisson distribution, with the expected number of traps depending on a specified uniform trap density and the volume of semiconductor material contained within the bounding box. You can also activate a special *single trap* mode, in which case, only one trap will be placed randomly within the semiconductor material contained within the bounding box.

You can run a statistical ensemble of trap configurations. When other sources of statistical variability (such as random discrete dopants) are activated, the entire ensemble of trap configurations will be run for each instance of the other statistical variability configurations. For example, if 200 devices with different RDD configurations are run with 1000 random SRH trap configurations, then a total of 200000 leakage currents will be calculated. Whether the same ensemble of trap configurations is run for each RDD configuration, or each list of trap positions is random, can be specified in the input file.

The input file command for random SRH traps is:

```
model random_srh_traps <parameter>=<value>
```

You activate the inclusion of random trap positions by setting `status=on`.

For descriptions of the parameters, see [Random Trap Positions on page 867](#).

The `single_trap` parameter controls whether the number of traps generated for each configuration follows a Poisson distribution based on the given trap density (`off`) or just one trap should be placed within the bounding box (`on`).

The ensemble of trap configurations can be set up by specifying the configuration number to start with (`start_config`) and the number of different configurations to use (`num_config`). Therefore, the trap configuration numbers that will be run go from `start_config` to (`start_config + num_config - 1`).

If you specify `repeat_config=on`, then the same list of trap configurations will be used for each statistical variability device configuration; otherwise, a different random list of trap configurations will be generated each time.

The parameter `trap_density` sets the uniform trap density that controls the expected number of traps when the single trap mode is not activated.

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### Additional Models

The energy level of the traps is set with the `trap_energy` parameter. If you do not set its value explicitly here, then the value used for the basic SRH model will also be used here.

You can include Gaussian variation in the trap energy by setting the standard deviation of that variation with the `trap_energy_sigma` parameter.

The trap cross-sections for electrons (`xsec_n`) and holes (`xsec_p`) control the generation rate following [Equation 35](#).

You can include Gaussian variation in the trap cross-sections by setting the standard deviation of that variation with the `xsec_n_sigma` and `xsec_p_sigma` parameters.

This variation is applied as a Gaussian on a log10 scale. Therefore, the standard deviation set with these parameters should be specified in decades.

The parameters `xmin`, `xmax`, `ymin`, `ymax`, `zmin`, and `zmax` define the bounding box within which the random traps will be placed. It is not necessary to specify all of these parameters because, by default, the bounding box extends to the maximum extent of the device structure in each direction. These limits are specified in nm unless the input units have been changed.

#### Note:

If any discrete traps are generated using this statistical method, then the contribution from each trap configuration to the overall leakage current will be calculated as a postprocess procedure after the general drift-diffusion solution. Any user-specified traps are also included automatically within each different trap configuration.

As the leakage from these traps is calculated as a postprocess, if a solution has been imported from a TDR file (see [Importing the Solution From Garand TDR Files](#)), then the trap leakage is still calculated even if Garand is set not to run a solution, that is, you have specified `simulation solve=off`.

## Traps on a Grid

When running in single trap mode, an option is available to place the trap on a grid of points within the bounding box, rather than completely randomly. This is useful when trying to map the parts of the device that are particularly sensitive to the presence of a trap, rather than doing a pure statistical analysis. To activate this option, use the command:

```
model random_srh_traps use_grid=on
```

A grid is overlaid on the structure and, for each point on the grid that is within the bounding box, Garand performs a leakage calculation, which considers a single trap at that point.

The resolution of the grid is 1 nm in each direction by default. This resolution, in nm, can be changed with the command:

```
model random_srh_traps grid_resolution=<float>
```

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This command sets the resolution in each direction to the same specified value. To change the resolution in a specific direction, you can set the `grid_resolution_x`, `grid_resolution_y`, and `grid_resolution_z` parameters individually to override the value set with `grid_resolution`, or its default value.

### Output

For each random trap configuration, the leakage current generated by the discrete traps will be calculated, along with the total current including the standard drift-diffusion current, the background SRH-generated current, and the current generated by the discrete traps. For each I–V bias point simulated, results will be written to a data file in the bias-dependent output directory. The file name will be:

```
<experiment>_random_trap_current_<device_number>.dat
```

where `<experiment>` is the simulation experiment name and `<device_number>` is the statistical-variability device number as specified by the `-d` option on the command line.

The file contains four columns of data:

- Trap configuration number
- Leakage current from solely the random traps
- Total drain current
- Number of traps in that configuration

When running in single trap mode, an additional CSV file is written that contains more information about the single trap. For each I–V bias point simulated, results are written to a data file in the bias-dependent output directory. The file name will be:

```
<experiment>_single_random_trap_data_<device_number>.csv
```

where `<experiment>` and `<device_number>` are as previously mentioned. The file has one line of comma-separated values per single trap configuration. On each line, there are the following values:

- Trap configuration number
- X-coordinate of the trap [nm]
- Y-coordinate of the trap [nm]
- Z-coordinate of the trap [nm]
- Leakage current solely from the random trap [A]
- Total drain current [A]
- Trap energy [eV]

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- Trap cross-section for electrons [cm<sup>2</sup>]
- Trap cross-section for holes [cm<sup>2</sup>]

## Leakage Calculation Based on an Imported Solution

As the leakage calculation is performed as a postprocess, it is not necessary to perform a full drift-diffusion solution in Garand if a suitable solution has been imported from a TDR file. This means that a solution that comes from Sentaurus Device can be used if the input TDR file has come from the output of Sentaurus Device, at the required bias conditions, and contains the necessary fields required to calculate the SRH leakage.

You need to set Garand so it will not perform a drift-diffusion solution by specifying:

```
simulation solve=off
```

You also need to activate the import of the solution contained in the TDR file using the command:

```
simulation import_solution=on
```

The fields that must be in the TDR file are:

- ElectrostaticPotential
- eDensity
- hDensity
- eQuasiFermiPotential
- hQuasiFermiPotential
- eQuantumPotential
- hQuantumPotential

#### Note:

As a solution is not performed in the Garand tool, the effect of variability sources such as random discrete dopants is not captured using this approach.

---

## Gate Leakage

Gate tunneling in a MOS structure is calculated using the Tsu–Esaki model [23] (first proposed by Duke [24]). The Tsu–Esaki tunneling formula expresses the gate leakage density by using an integration in the energy domain. This model allows separation of the tunneling current between the supply function, which describes the supply of carriers ready for tunneling at each energy level, and the transmission coefficient seen by each wave packet through the considered energy barrier. The supply function depends on the carrier

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### Additional Models

energy distribution adopted in the simulation (such as Maxwell–Boltzmann or Fermi–Dirac). The transmission coefficient can be found by a solution of a 1D Schrödinger equation in the MOS gate stack structure.

In Garand, the WKB approximation [25] is adopted in the calculation of the barrier transparency, although more refined methods such as the transfer matrix method [26] and the quantum transmitting boundary method [27] can be implemented. It is worth noting that, in the channel of an inverted MOSFET, the strong band bending at the channel–oxide interface leads to the creation of a quasi-triangular quantum well with eigenfunctions that have bound and quasi-bound states. The former do not contribute to the tunneling process, while the latter can contribute to additional gate leakage. Garand neglects the contribution of quasi-bound states to the gate tunneling.

In the Tsu–Esaki formalism, the net leakage through the oxide reads as:

$$J_{\text{net, leakage}} = J_{s \rightarrow g} - J_{g \rightarrow s} \quad (38)$$

where:

$$\begin{aligned} J_{s \rightarrow g} &= \frac{4q\pi m_{s,\text{eff}}}{h^3} \int_{E_{\min}}^{E_{\max}} T(E_{\perp}) dE_{\perp} \int_0^{\infty} f_s(E)(1-f_g(E)) dE_{\parallel} \\ J_{g \rightarrow s} &= \frac{4q\pi m_{g,\text{eff}}}{h^3} \int_{E_{\min}}^{E_{\max}} T(E_{\perp}) dE_{\perp} \int_0^{\infty} f_g(E)(1-f_s(E)) dE_{\parallel} \end{aligned} \quad (39)$$

Here,  $g$  refers to the gate and  $s$  refers to the substrate. The total integration is performed over the energy component perpendicular to the tunneling interface, while the supply function (a measure of the number of carriers ready for tunneling and having the velocity vector in the direction perpendicular to the interface) is calculated by performing an integral over the energy component parallel to the tunneling interface. The different masses corresponding to the band structure of the gate-stack materials (gate electrode, dielectric, and substrate) are lumped into a single effective mass value. You define these values, as specified by the input parameters (see [Gate Leakage Model on page 870](#)).

In this calculation, Garand considers the carrier energy distribution to always be a Fermi–Dirac distribution on both the electrode and substrate sides.

The barrier transparency (or transmission coefficient)  $T$  is defined as the ratio between the quantum-mechanical current density due to an incident wave before the barrier and a transmitted wave after the barrier and, under the WKB approximation can be expressed as:

$$T(E_{\perp}) = \exp\left(\int_{x_1}^{x_2} \sqrt{2m_{\text{ox, eff}}(W_{\perp}(x) - E_{\perp}(x))} dx\right) \quad (40)$$

where the integration is performed only between the classical turning points  $x_1$  and  $x_2$  where the perpendicular electron energy  $E_{\perp}(x)$  is lower than the perpendicular barrier profile  $W_{\perp}(x)$ , so that the integral is always real.

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This tunneling model is applied along each 1D path perpendicular to the local semiconductor–oxide interface (defined according to the simulation mesh). Therefore, the model is suitable for calculating the gate leakage for complex nonplanar gate structures such as FinFETs and nanowire transistors.

Finally, it is important to emphasize that, in the presence of oxide defects, trap-assisted tunneling can represent a major contribution to gate leakage, especially at low electric fields. A trap-assisted tunneling model is included in the calculation of gate leakage according to [28][29], and you can specify trap density in the oxide, the trap capture cross-section, and the attempt-to-escape frequency by using the input parameters.

To switch on a gate leakage simulation, use the following command:

```
model gate_leakage status=on <parameter>=<value>
```

For details about the parameters, see [Gate Leakage Model on page 870](#).

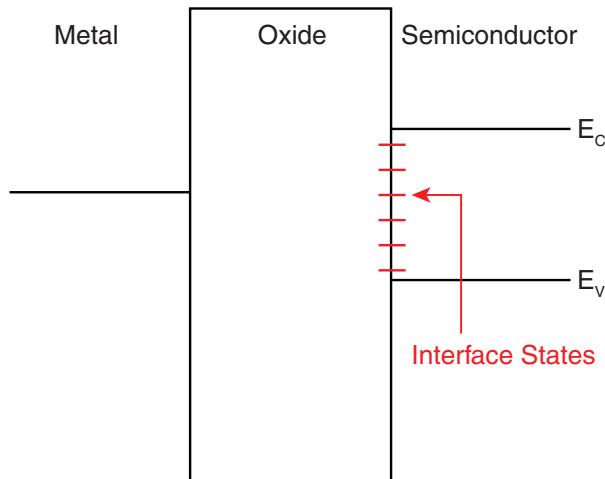
---

## Interface Charge

You can include interface charge due to traps in the drift-diffusion simulation of the electrical behavior of a MOS transistor. These defects are located at the semiconductor–oxide interface with energy distributions within the semiconductor band gap.

Electrons or holes can be trapped in these states, thereby modifying the electrostatic behavior of the transistor. [Figure 25](#) shows a schematic band diagram of a MOSFET including localized interface traps.

*Figure 25 Schematic band diagram of a MOSFET including interface traps*



The probability that an electron or a hole occupies a given interface state depends on the energetic location of the state relative to the Fermi level in the semiconductor. The energy

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### Additional Models

level of the interface states is fixed with respect to the semiconductor band edges at the interface. Therefore, the occupation probability of the interface states changes according to the relative position of the Fermi level with respect to the defect energy level. In particular, for a given value of the surface potential  $\varphi_s$ , the net sheet charge density in the interface traps can be calculated by:

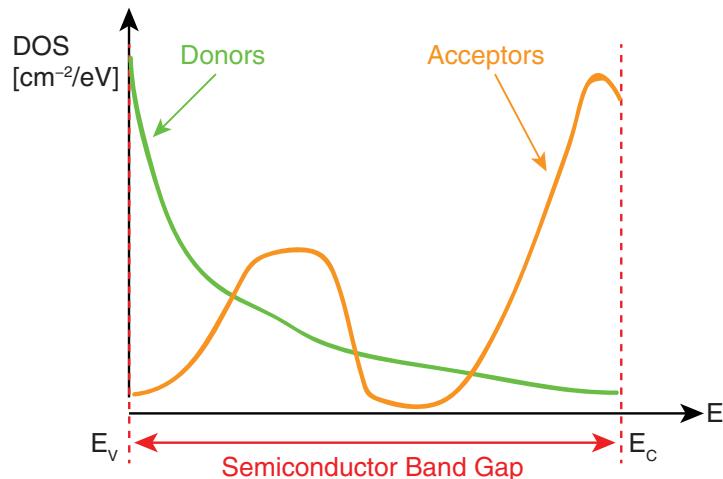
$$Q_{it}(\varphi_s) = q \int_{E_g} \{ [1 - f(\varepsilon)] D_{it}^D(\varepsilon) - f(\varepsilon) D_{it}^A(\varepsilon) \} d\varepsilon \quad (41)$$

where the dependence from  $\varphi_s$  is hidden in the relative position of the Fermi distribution  $f$  with respect to the density of *donor interface traps*  $D_{it}^D$  and *acceptor interface traps*  $D_{it}^A$ . In this respect, the conventional use of terms is adopted:

- If a state is neutral and become positively charged when accepting a hole, it is called a *donor* state.
- If a state is neutral and become negatively charged when accepting an electron, it is called an *acceptor* state.

[Figure 26](#) shows a schematic example of interface trap distributions.

*Figure 26 Illustration of distributions of donor and acceptor density of traps at the semiconductor–oxide interface*



The recommended way to define interface charge distributions is using an analytic function as described in [Analytic Interface Charge Distributions on page 153](#).

However, the legacy method of supplying charge distributions in a file is still available. You can specify both donor and acceptor distributions in a file with the following three-column format:

- Column 1: Energy (eV) above the valence band edge

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- Column 2: Sheet density ( $\text{cm}^{-2}/\text{eV}$ ) for donor-type traps at this energy level
- Column 3: Sheet density ( $\text{cm}^{-2}/\text{eV}$ ) for acceptor-type traps at this energy level

#### Example: Trap Density Distribution for Silicon

# E [eV]	donor [ $\text{cm}^{-2}/\text{eV}$ ]	acceptor [ $\text{cm}^{-2}/\text{eV}$ ]
0.00	1.00000E+13	1.31170E+08
0.02	8.18731E+12	1.60212E+08
0.04	6.70320E+12	1.95683E+08
0.06	5.48812E+12	2.39008E+08
.	.	.
.	.	.
.	.	.
1.08	2.03995E+08	6.43007E+12
1.10	1.67017E+08	7.85370E+12
1.12	1.36742E+08	9.59253E+12
1.14	1.11955E+08	1.17163E+13

#### Note:

The amount of trapped charge in [Equation 41](#) depends on the surface potential  $\phi_s$ , which depends on the amount of trapped charge as ruled by the Poisson equation. Therefore, in Garand, [Equation 41](#) is solved iteratively with the Poisson equation, until this coupled scheme converges.

Because the occupation of these interface states responds to variation of the surface potential, the inclusion of these defects in the drift-diffusion simulation results in deformations of the MOS capacitance–voltage (C–V) curves and degradation of the subthreshold slope in the MOS transfer characteristics.

To switch on an interface traps simulation, use the following command:

```
model interface_charge <parameter>=<value>
```

You must provide the material in which the interface traps will be modeled and the name of the file that contains the trap distributions in the three-column format previously described. For example:

```
model interface_charge status=on material=silicon \
    file='trap-dist-si.dat'
model interface_charge status=on material=si40ge60 \
    file='trap-dist-si40ge60.dat'
```

#### Note:

You can include multiple `model interface_charge` commands in the input file for specifying multiple materials in which to include the interface charge.

For details about the parameters, see [Interface Charge Model on page 871](#).

## Analytic Interface Charge Distributions

The recommended way to include interface traps is by defining interface trap distribution models. You use the `define` command to define an interface model, with the following general syntax:

```
define <material1>.<material2>.<interface> <interface_model>
```

where:

- `<material1>` and `<material2>` are the unique names of the materials, or regions, that form the interface.
- `<interface>` is a unique user-defined name to identify the interface model.
- `<interface_model>` is a keyword that specifies the model to be defined. Options are:
  - `trap_exponential`: [Exponential Interface Trap Distribution on page 155](#)
  - `trap_gaussian`: [Gaussian Interface Trap Distribution on page 155](#)
  - `trap_level`: [Discrete Interface Trap Level Model on page 156](#)
  - `trap_table`: [Tabulated Interface Trap Distribution on page 157](#)
  - `trap_uniform`: [Uniform Interface Trap Distribution on page 158](#)

**Note:**

You can include an interface charge only at the interface between a semiconductor and an insulator.

## Common Parameters of Interface Charge Distribution Models

All interface charge distribution models define a set of parameters that can be assigned in the input file by using the `interface` command with the following general syntax:

```
interface <material1>.<material2>.<interface>.<parameter> <value>
```

where:

- `<material1>` and `<material2>` are the unique names of the materials, or regions, that form the interface.
- `<interface>` is the name of a previously defined interface model between `<material1>` and `<material2>`.
- `<parameter>` is a parameter associated with the model.
- While the set of parameters differs for different models, all models define the parameters in [Table 4](#).

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### Additional Models

**Table 4** Parameters common to interface charge distribution models

Parameter	Description	Type	Default
carrier	Sets the carrier type to which the interface model is tied. Options are: <ul style="list-style-type: none"><li>• electrons</li><li>• holes</li></ul>	string	—
DLN	Sets the number of discrete levels over which the trap distribution is integrated. The energy levels span the valence band edge to the conduction band edge, separated into 13 steps by default.	integer	13
orient	Sets the $\langle hkl \rangle$ crystal orientation of the interface and ties a model to a specific orientation.	vector	—
type	Mandatory. Specifies whether traps are donor like or acceptor like. If you do not specify this parameter, then an error is generated. Options are: <ul style="list-style-type: none"><li>• acceptor</li><li>• donor</li><li>• eneutral</li><li>• fixedcharge</li><li>• hneutral</li></ul> <p>Use <code>acceptor</code> or <code>eneutral</code> to define the trap level as acceptor-like. Use <code>donor</code> or <code>hneutral</code> to define the trap level as donor-like. In these cases, the occupation of traps is calculated by using the Fermi–Dirac occupation function.</p> <p>You can specify <code>fixedcharge</code>, in which the traps are always occupied, with the sign of the trap density in subsequent models determining if they are donor-like or acceptor-like.</p>	string	—

The orientation (`orient`) is not mandatory. If not set, the interface model matches all interfaces between the two named materials found within the domain. If set, the model matches only interfaces between the two named materials in the domain with the same orientation. If multiple interface models of the same type are defined between the same two materials, then the model that explicitly matches an interface in the simulation domain takes priority. If an exact match is not found, then the general orientation-independent model is used.

The `carrier` parameter ties the interface model to a specific carrier, which can be useful for calibration where different values might give better results for different carriers. The `carrier` parameter is not mandatory. If not set, the interface model matches both carriers. If set, it must be set to either `electrons` or `holes`, and the model matches only when that carrier is

## Chapter 3: Simulation Setup

### Additional Models

simulated. If multiple interface models of the same type are defined between the same two materials, then the model that explicitly matches the carrier being simulated takes priority. If an exact match is not found, the general carrier-independent model is used.

## Exponential Interface Trap Distribution

An exponential interface trap distribution model allows the association of parameters that describe an exponential distribution of traps over an energy range at an interface.

As well as the parameters common to all interface trap distribution models (see [Table 4](#)), a `trap_exponential` model defines the parameters in [Table 5](#).

*Table 5 Parameters specific to trap\_exponential model*

Parameter	Description	Type	Default	Unit
<code>E0</code>	Sets the energy of the midpoint of the energy distribution relative to the valence band edge.	float	0.0	eV
<code>Es</code>	Sets the width of the energy range over which the trap density is defined.	float	0.0	eV
<code>N0</code>	Sets the magnitude of the trap density, such that the density $N(E) = N0 \exp\left(-\frac{E - E0}{Es}\right)$ .	float	0.0	$\text{cm}^2 \text{eV}^{-1}$

### Example

Define an exponential interface trap distribution model called `level` between Silicon and Oxide:

```
define Silicon.Oxide.level trap_exponential
interface Silicon.Oxide.level.type acceptor      # Acceptor traps
interface Silicon.Oxide.level.E0    0.5 # Energy above valence band [eV]
interface Silicon.Oxide.level.Es    0.4 # Energy range about E0 [eV]
interface Silicon.Oxide.level.N0   1.0E10 # Peak trap density [/cm2 /eV]
```

As the `orient` and `carrier` parameters are not set, this definition will match all interfaces for both electrons and holes.

## Gaussian Interface Trap Distribution

A Gaussian interface trap distribution model allows the association of parameters that describe a Gaussian distribution of traps over an energy range at an interface.

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### Additional Models

As well as the parameters common to all interface trap distribution models (see [Table 4](#)), a `trap_gaussian` model defines the parameters in [Table 6](#).

*Table 6 Parameters specific to trap\_gaussian model*

Parameter	Description	Type	Default	Unit
E0	Sets the energy of the midpoint of the energy distribution relative to the valence band edge.	float	0.0	eV
Es	Sets the width of the energy range over which the trap density is defined.	float	0.0	eV
N0	Sets the magnitude of the trap density, such that the density is: $N(E) = N0 \exp\left(-\frac{(E - E0)^2}{2Es^2}\right)$	float	0.0	cm <sup>2</sup> eV <sup>-1</sup>

### Example

Define a Gaussian interface trap distribution model named `level` between Silicon and Oxide:

```
define    Silicon.Oxide.level trap_gaussian
interface Silicon.Oxide.level.type hneutral # Donor traps
interface Silicon.Oxide.level.E0    0.9    # Energy above valence band [eV]
interface Silicon.Oxide.level.Es    0.2    # Energy range about E0 [eV]
interface Silicon.Oxide.level.N0    1.0E10 # Peak trap density [/cm2 /eV]
```

As the `orient` and `carrier` parameters are not set, this definition will match all interfaces for both electrons and holes.

## Discrete Interface Trap Level Model

An interface trap level model allows the association of parameters that describe the density of traps at a single energy level at an interface. Parameters are assigned in the input file using the `interface` command as with all interface models.

As well as the parameters common to all interface trap distribution models (see [Table 4](#)), a `trap_level` model defines the parameters in [Table 7](#).

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Table 7 Parameters specific to trap\_level model

Parameter	Description	Type	Default	Unit
E0	Sets the energy of the trap relative to the valence band edge.	float	0.0	eV
N0	Sets the magnitude of the trap density, such that the density $N(E) = N0$ for $E = E0$ .	float	0.0	cm <sup>2</sup>

### Example

Define an interface trap level model named level between Oxide and HfO<sub>2</sub>:

```
define Oxide.HfO2.level trap_level
interface Oxide.HfO2.level.type donor      # Donor traps
interface Oxide.HfO2.level.E0    0.2        # Energy above valence band [eV]
interface Oxide.HfO2.level.N0    5.0E10     # Trap density [/cm3]
```

As the orient and carrier parameters are not set, this definition will match all interfaces for both electrons and holes.

## Tabulated Interface Trap Distribution

A tabulated interface trap distribution model allows the association of parameters that describe a user-defined distribution of traps in energy at an interface.

As well as the parameters common to all interface trap distribution models (see [Table 4 on page 154](#)), a trap\_table model defines the parameter in [Table 8](#).

Table 8 Parameter specific to trap\_table model

Parameter	Description	Type	Default	Unit
table	Sets a list of energy and density value pairs (eV, cm <sup>2</sup> eV <sup>-1</sup> ) that together define the distribution, such that the density $N(E) = N_i$ for $E_{i-1} < E \leq E_{i+1}$ .	table	(0.0, 0.0)	—

### Example

Define a tabulated interface trap distribution model named level between Silicon and Oxide:

```
define Silicon.Oxide.level trap_table
interface Silicon.Oxide.level.type hneutral      # Donor traps
interface Silicon.Oxide.level.table E 0.00 piecewise 0.0E11
```

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```
# 0.0 eV -> 0.1 eV
interface Silicon.Oxide.level.table E 0.10 piecewise 1.0E11
# 0.1 eV -> 0.2 eV
interface Silicon.Oxide.level.table E 0.20 piecewise 5.0E11
# 0.2 eV -> 0.3 eV
interface Silicon.Oxide.level.table E 0.30 piecewise 1.0E11
# 0.3 eV -> 0.4 eV
interface Silicon.Oxide.level.table E 0.40 piecewise 0.0E11 # 0.4 eV ->
```

As the `orient` and `carrier` parameters are not set, this definition will match all interfaces for both electrons and holes.

## Uniform Interface Trap Distribution

A uniform interface trap distribution model allows the association of parameters that describe a uniform distribution of traps over an energy range at an interface.

As well as the parameters common to all interface trap distribution models (see [Table 4 on page 154](#)), a `trap_uniform` model defines the parameters in [Table 9](#).

*Table 9 Parameters specific to trap\_uniform model*

Parameter	Description	Type	Default	Unit
E0	Sets the energy of the midpoint of the energy distribution relative to the valence band edge.	float	0.0	eV
Es	Sets the energy range over which the trap density is defined.	float	0.0	eV
N0	Sets the magnitude of the trap density, such that the density $N(E) = N_0$ for $E - \frac{1}{2}Es < E0 < E + \frac{1}{2}Es$ .	float	0.0	$\text{cm}^2 \text{eV}^{-1}$

## Example

Define a uniform interface trap distribution model named `level` between `Silicon` and `Oxide`:

```
define Silicon.Oxide.level trap_uniform
interface Silicon.Oxide.level.type acceptor # Acceptor traps
interface Silicon.Oxide.level.E0 0.5 # Energy above valence band [eV]
interface Silicon.Oxide.level.Es 0.4 # Energy range about E0 [eV]
interface Silicon.Oxide.level.N0 1.0E10 # Trap density [/cm2 /eV]
```

As the `orient` and `carrier` parameters are not set, this definition will match all interfaces for both electrons and holes.

## Random Dopant Mobility Variation

Traditionally, in drift-diffusion simulations, the variation in device characteristics is purely a result of electrostatic variations due to discrete dopants. There is no accounting for variation in mobility and, as such, variation in the on-current might be underestimated. To account to some degree for this mobility variation, a model is available that can modify the mobility due to ionized impurity scattering based on the number of discrete dopants in the channel of the device.

You must specify an appropriate region within the channel where the number of channel dopants (that is, acceptors in n-type MOSFETs or donors in p-type MOSFETs) is counted and an averaged channel doping is calculated as:

$$N_{av} = \frac{N}{V} \quad (42)$$

where:

- $N_{av}$  is the averaged channel doping concentration in  $\text{cm}^{-3}$ .
- $N$  is the number of discrete dopants in the specified region.
- $V$  is the volume of the specified region in  $\text{cm}^3$ .

When calculating the low-field mobility based on the doping concentration at a mesh node, the value of  $N_{av}$  is used within the defined region rather than the nominal uniform doping concentration.

The model is specified with the command:

```
model rdd_mobility <parameter>=<value>
```

For descriptions of the parameters, see [Variation in Random Dopant Mobility on page 872](#).

**Note:**

It is not necessary to specify all bounding box limits (`xmin`, `xmax`, and so on) as they will default to the maximum extent of the simulation domain in that direction.

---

## Numeric Solution

The basis of Garand is the solution of the quantum-corrected drift-diffusion system of partial differential equations, namely, the Poisson equation, the density gradient equation, and the current continuity equation for the majority carriers.

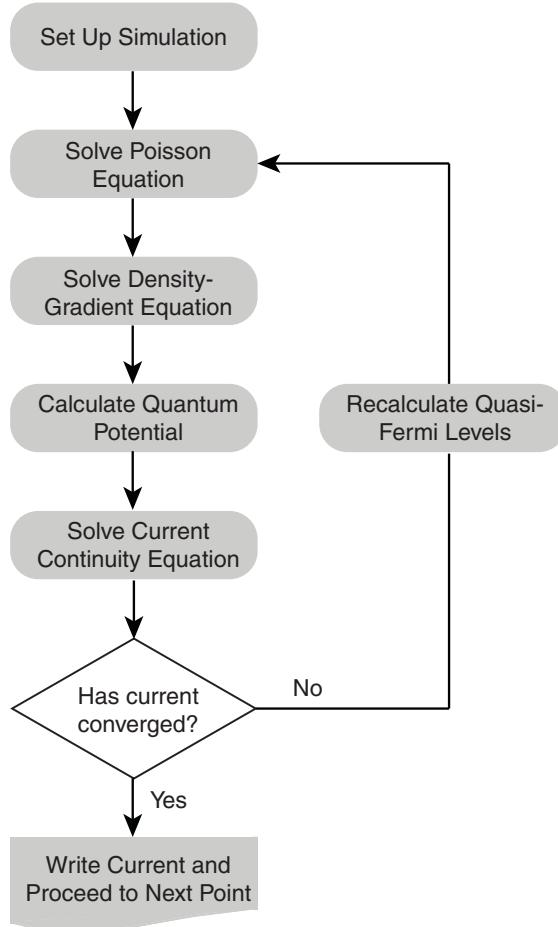
This set of equations must be solved self-consistently to obtain the electrostatic potential and the quantum-corrected carrier distribution. The discussion here assumes that an n-type MOSFET is being simulated; the solution for a p-type device is analogous.

## Modified Gummel Decoupled Method

Garand uses the Gummel decoupled method for the self-consistent solution of this system of equations. This method is modified to include the solution of the density gradient equation. In this approach, each equation is solved in turn, with the result of each solution feeding into the solution of the next equation, and the process is repeated until the system is self-consistent. This is illustrated diagrammatically in [Figure 27](#).

After the simulation domain is set up by specifying the mesh (as in [Specifying a Mesh on page 52](#)) and the doping profiles (as in [Doping Profiles on page 63](#)), each partial differential equation (PDE) is discretized on the simulation mesh to produce a set of algebraic equations, the unknowns of which are the discrete values of the continuous variables at the mesh nodes. Finally, the large set of algebraic equations (one equation for each node in the grid) must be solved to produce a discrete approximation to the continuous solution of each PDE.

*Figure 27 Flow of the solution of the coupled set of equations*



## Chapter 3: Simulation Setup

### Numeric Solution

## Poisson Equation

The Poisson equation is:

$$\nabla \cdot (\epsilon \nabla \psi) = -q(p - n + N_D^+ - N_A^-) \quad (43)$$

For example, considering the Poisson equation ([Equation 43](#)), the discretization gives an algebraic equation of the form:

$$a\psi_{i-1,j,k} + b\psi_{i,j-1,k} + c\psi_{i,j,k-1} + d\psi_{i,j,k} + e\psi_{i,j,k+1} + f\psi_{i,j+1,k} + g\psi_{i+1,j,k} = Q \quad (44)$$

for each node in the simulation mesh. This relates the electrostatic potential at that node  $(i, j, k)$  to the potential at the six neighboring nodes through the coefficients  $a$  to  $g$ . Those coefficients are specific to that node, and each node will have its own set of different coefficients.

When all of the algebraic equations are combined, they form a system of equations that can be considered a matrix equation of the form:

$$A \cdot x = b \quad (45)$$

where:

- $A$  is the discretization matrix, which is a seven-diagonal matrix formed by all the above coefficients where each line of the matrix represents the algebraic equation for one mesh node.
- $x$  is the unknown vector for which the matrix equation must be solved. This consists of the potential,  $\psi$ , at each mesh node.
- The right-hand side vector,  $b$ , is the discretized right-hand side term of the Poisson equation and is effectively the net amount of charge at each node.

[Figure 28](#) shows the full matrix equation.

The Poisson equation ([Equation 43](#)) is solved to obtain the electrostatic potential,  $\psi$ . The electron concentration,  $n$ , depends on  $\psi$  through the carrier statistics (Maxwell–Boltzmann or Fermi–Dirac) and this dependence must be accounted for when solving the Poisson equation. Unfortunately, this results in a nonlinear system. Therefore, it is not sufficient to solve a linear system such as in [Equation 45](#).

The nonlinear system must be linearized using a Newton method and the resultant linear system must be solved. This linearization and solution must be repeated until the point where further linearization does not result in a significantly different solution.

In the actual solution of the nonlinear Poisson equation in Garand, a Newton successive over-relaxation (SOR) [\[30\]](#)[\[31\]](#) solver is used, where the linearization is applied every  $n$  iterations of the SOR solver, where  $n$  is 50 by default.

The value of  $n$  can be changed with the command:

```
simulation poisson_nonlinear_update=<integer>
```

## Chapter 3: Simulation Setup

### Numeric Solution

When including the density gradient equation in the Gummel loop, the boundary conditions used for the Poisson equation are Neumann boundary conditions, which allow the electrostatic potential to float so it will be consistent with the quantum-corrected carrier distribution. To force a fixed Dirichlet boundary condition for the Poisson solution, include the command:

```
contact sd_boundary = dirichlet
```

**Figure 28** Full matrix equation showing the seven-diagonal structure of the finite difference discretization

$$\begin{bmatrix} d_1 & e_1 & & f_1 & & g_1 \\ c_2 & d_2 & e_2 & f_2 & & g_2 \\ c_3 & d_3 & e_3 & f_3 & & g_3 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \\ a_i & & b_i & c_i & d_i & e_i & f_i & g_i \\ \vdots & & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{n-2} & & b_{n-2} & c_{n-2} & d_{n-2} & e_{n-2} & f_{n-2} & g_{n-2} \\ a_{n-1} & & b_{n-1} & c_{n-1} & d_{n-1} & e_{n-1} & f_{n-1} & g_{n-1} \\ a_n & & b_n & c_n & d_n & & & \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \\ \psi_i \\ \vdots \\ \psi_{n-2} \\ \psi_{n-1} \\ \psi_n \end{bmatrix} = \begin{bmatrix} Q_1 \\ Q_2 \\ Q_3 \\ \vdots \\ Q_i \\ \vdots \\ Q_{n-2} \\ Q_{n-1} \\ Q_n \end{bmatrix}$$

The diagram illustrates the seven-diagonal structure of a finite difference discretization. The matrix is a sparse matrix with non-zero entries forming seven diagonals around the main diagonal. The diagonals are labeled with coefficients:  $d_i$ ,  $e_i$ ,  $f_i$ ,  $g_i$  along the main diagonal;  $a_i$ ,  $b_i$ ,  $c_i$ ,  $d_i$ ,  $e_i$ ,  $f_i$ ,  $g_i$  along the super-diagonals; and  $a_{n-1}$ ,  $b_{n-1}$ ,  $c_{n-1}$ ,  $d_{n-1}$ ,  $e_{n-1}$ ,  $f_{n-1}$ ,  $g_{n-1}$  along the sub-diagonals. Arrows indicate the width of the diagonals:  $n_z$  for the vertical extent of the super-diagonals,  $n_z \times ny$  for the horizontal extent of the super-diagonals, and  $n_z$  for the vertical extent of the sub-diagonals.

## Density Gradient Equation

The density gradient equation is:

$$2b_n \frac{\nabla^2 \sqrt{n}}{\sqrt{n}} c = \phi_n - \psi + \frac{k_B T}{q} \ln\left(\frac{n}{n_f}\right) \quad (46)$$

The density gradient equation (Equation 46) is considered in the anisotropic form given in [Equation 4 on page 123](#) and is discretized and solved in terms of  $S = \sqrt{n}$ , from which the

## Chapter 3: Simulation Setup

### Numeric Solution

quantum-corrected electron concentration,  $n$ , is obtained. This equation is also nonlinear and is solved using the Newton SOR solver.

The effective quantum-corrected potential is then calculated from:

$$\psi_{\text{eff}} = \psi + 2b_n \frac{\nabla^2 \sqrt{n}}{\sqrt{n}} = \phi_n + \frac{k_B T}{q} \ln\left(\frac{n}{n_i}\right) \quad (47)$$

By default, the solution of the density gradient equation is included in the Gummel iterative cycle starting at the first iteration. You can delay the inclusion of the density gradient solution, so that it starts at a later iteration, which can sometimes help the stability of the solution of the overall coupled system. To specify the iteration at which the inclusion of the density gradient solution should start, use the command:

```
simulation dg_start_iter=<integer>
```

## Current Continuity Equation

The effective quantum-corrected potential is then used as the driving potential for the current continuity equation:

$$\nabla \cdot J_n = 0 \quad (48)$$

which is solved to account for the electron transport under the influence of the quantum-corrected electric field.

Only the majority-carrier continuity equation needs to be solved for the unipolar CMOS devices that Garand is designed to simulate, so the net generation–recombination rate can be assumed to be zero.

In the quantum-corrected drift-diffusion approximation, in [Equation 48](#),  $J_n$  is given by:

$$J_n = -qn\mu_n \nabla \psi_{\text{eff}} + qD_n \nabla_n \quad (49)$$

The solution of [Equation 48](#) employs a standard Scharfetter–Gummel discretization [32][33] that is modified to use the quantum-corrected potential from [Equation 47](#) as the driving force rather than the normal classical potential.

The right-hand side of [Equation 48](#) is zero, so the matrix equation that is formed by the discretization of the current continuity equation is linear. This linear system is solved for the electron density,  $n$ , using a bi-conjugate gradient stabilized (Bi-CGSTAB) solver [34].

The system of equations [Equation 43](#), [Equation 46](#), and [Equation 48](#) is solved successively and repeatedly until self-consistent convergence is achieved. Convergence is assessed on the change in the current through the device calculated on successive Gummel iterations. If the change in current is less than the tolerance specified in the input file (`simulation gummel_acc=<float>`), then the simulation is considered to have reached self-consistent convergence.

## Chapter 3: Simulation Setup

### Numeric Solution

To determine the current through the device, the calculated current densities at each node must be integrated over a surface that encloses the drain contact. The surface that is integrated over can affect the stability and convergence of the simulation as this is based on the convergence of the current.

#### Alternative Current Integration Method

Garand attempts to optimize the surface used and, for standard device architectures (such as planar bulk MOSFET and FDSOI, and FinFET), this is generally reliable. However, for more novel architectures, it might not be optimal. An alternative method is available to set the current integration surface that can provide more stable results in some devices.

To select the method to use, specify the command:

```
simulation current_integration=<integer>
```

where 1 selects the default method and 2 selects the alternative method. If the simulation is exhibiting convergence problems, then try the other current integration method.

---

## Input File Options

You can specify the tolerances to which the Gummel iteration, the PDE solutions, and so on must be solved in the input file. The default values give reliable results in most cases; however, you can modify these if there are convergence problems in the solution.

Various numeric solution parameters can be modified by using the `simulation` command. For descriptions of the parameters, see [simulation Command on page 884](#).

The `solve` parameter specifies whether to obtain a full drift-diffusion solution, or to solve only the nonlinear Poisson equation, or to have no solution. If the drift-diffusion equations are not solved, Garand will execute the device setup and initialization, and this initial state will be written as output. This is useful for testing the device description and importing doping profiles without having to wait for a solution to be obtained.

There is also the `poisson` option that specifies to perform only a single solution of the nonlinear Poisson equation. This can be used to obtain the classical equilibrium potential distribution (that is, with no applied drain bias). An equilibrium quantum-corrected solution can be obtained by specifying `solve=dg` with zero applied bias. This will iteratively solve the Poisson and density gradient equations until a self-consistent solution is achieved.

The accuracy that must be used to test for the convergence of the Gummel iterations is specified with `gummel_acc`. The quantity tested is the relative change in the device current from the last iteration to the present iteration, that is,  $\Delta I = |I_n - I_{n-1}| / I_{n-1} < \text{gummel\_acc}$ , where  $n$  is the current Gummel iteration. It also requires the change from the second-to-last iteration to the present iteration to also fall within this tolerance, to improve confidence in the determination of convergence.

## Chapter 3: Simulation Setup

### Numeric Solution

When you specify `solve=dg`, the current continuity equation is not solved, only the nonlinear Poisson equation and the density gradient equation. These are solved iteratively, as in the normal Gummel loop, but no current is calculated. Two convergence tests are used:

- One test is based on the change in potential.

For the potential test, the change in potential at each mesh node from one ‘Gummel’ iteration to the next must be lower than the specified tolerance given by `poisson_qc_acc`.

- One test is based on the change in  $\log_{10}$  of the carrier concentration.

For the carrier concentration test, the change in  $\log_{10}$  of the carrier concentration at each mesh node from one ‘Gummel’ iteration to the next must be lower than the same tolerance. However, in this case, only nodes in the semiconductor where the carrier concentration is greater than  $1 \text{ cm}^{-3}$  are considered.

If either convergence test is passed, then the system is considered to have converged and the simulation stops.

The solvers used to solve the Poisson, the current continuity, and the density gradient equations each determine convergence by checking the average relative change over the *entire* mesh of the quantity being solved for. For convergence, this relative change must be smaller than the tolerance specified by `espois`, `epscurr`, and `epsdg`, respectively. However, due to the decoupled iterative Gummel method used to achieve overall self-consistent solutions, it is not necessary to solve these separate PDEs to full convergence at each Gummel iteration, and doing so is often inefficient and unnecessarily time-consuming. For this reason, you can limit the number of iterations that each solver performs. You specify these limits with `nlimitp`, `nlimitc`, and `nlimitdg` for the Poisson, the current continuity, and the density gradient equations, respectively.

It is still the objective in the final Gummel iteration of the simulation that each PDE solution converges within its respective iteration limits. The `pot_converged` parameter controls whether the Poisson solution must converge fully before the Gummel cycle can be considered to be converged and it is switched off by default.

You use the `iter_min` parameter to specify the minimum number of Gummel iterations that must be performed. In general, it should not be necessary to use this parameter. However, occasionally when running an  $I_d$ – $V_d$  simulation, you might observe that the simulator meets the specified convergence criterion for the current after only a few Gummel iterations, and that the current has not changed significantly from the last I–V point. This false convergence is due to the fact that it can take several iterations for the full effect of the change of drain boundary conditions to be propagated through the simulation domain and to be observed in the calculated current. In this case, it is prudent to specify a minimum number of Gummel iterations (15 to 20 is usually sufficient) to avoid false convergence.

## Output

This section discusses how to generate output files for drift-diffusion simulations.

---

### Output Files

The main output from simulations is I–V data, written to a .dat file. You can customize the file output by specifying an experiment name and the output directory using the `output` command. For example:

```
output experiment='bulk-nmos'  
output directory='path_to_folder'
```

For descriptions of the parameters discussed in this section, see [output Command on page 873](#).

When Garand runs an I–V simulation, the results are written to the file:

```
<experiment>_IdVg_Vd<drain_bias>_Vsub<substrate_bias>_<device_number>.dat  
for an Id–Vg curve with Vd=<drain_bias> and Vsub=<substrate_bias> or:  
<experiment>_IdVd_Vg<gate_bias>_Vsub<substrate_bias>_<device_number>.dat  
for an Id–Vd curve with Vg=<gate_bias> and Vsub=<substrate_bias> or:  
<experiment>_Target_Vd<drain_bias>_Vsub<substrate_bias>_<device_number>.dat  
for a target current search with Vd=<drain_bias> and Vsub=<substrate_bias>.
```

Here, <device\_number> is the number of the device within a statistical ensemble specified by the `-d` command-line option (default is 1).

If a substrate contact is not present, then the substrate bias is not appended to the I–V file name. For example:

```
<experiment>_IdVg_Vd<drain_bias>_<device_number>.dat
```

The I–V file contains multiple columns of output. The first column is the gate or drain voltage (in V), and the other columns are the different contact currents (in A). You can deactivate writing results to a .dat file with the command:

```
output dat=off
```

#### Note:

If you are not simulating an entire device structure, then see [Scaling the Output Current on page 74](#) for information about how to scale the output current by specifying an area factor.

## Chapter 3: Simulation Setup

### Output

Garand also writes I–V and C–V data in PLT format that can be read by Sentaurus Visual, which can then plot the output. The files are written to the same location and with the same file names, as the .dat files previously described, but with the .plt file extension instead. You can deactivate writing results to a .plt file with the command:

```
output plt=off
```

You can also write the output I–V data to a comma-separated values (.csv) file. This type of data file can also be read by Sentaurus Visual or the Microsoft® Excel® application. To activate CSV output, include the command:

```
output csv=on
```

---

## Output File for Visualization

For postprocess visualization using Sentaurus Visual, a TDR output file must be written. Parameters for generating a TDR file are specified by using the `output` command:

```
output <parameter>=<value>
```

For details about visualization-specific parameters, see [output Command on page 873](#).

A TDR file is written for every I–V point simulated. Garand writes the output TDR file into a subdirectory named `viz` within a bias-dependent output directory named with the  $V_d$  and  $V_g$  bias conditions unless you specify `output hierarchical=off` (see [Hierarchy of the Output Directory on page 188](#)). The TDR file is labeled with the device number within the statistical ensemble (1 by default). For example:

```
<experiment>-DD-Output_<device_number>.tdr
```

You can specify the units used for distances in the output, such as device dimensions in the TDR file and distances in cutlines. By default, all output is in micrometers, to be consistent with other Synopsys tools, allowing comparison with the input TDR file that will be in micrometers. To change the unit of the output to be nanometer, use the command:

```
output units = nm
```

By default, some quantities such as mobility, bands, and Fermi level are written to the TDR file. However, you can exclude these quantities, thereby reducing the file size.

To exclude these quantities from the TDR file, use the following commands:

```
output mobility = off  
output bands     = off  
output fermi     = off
```

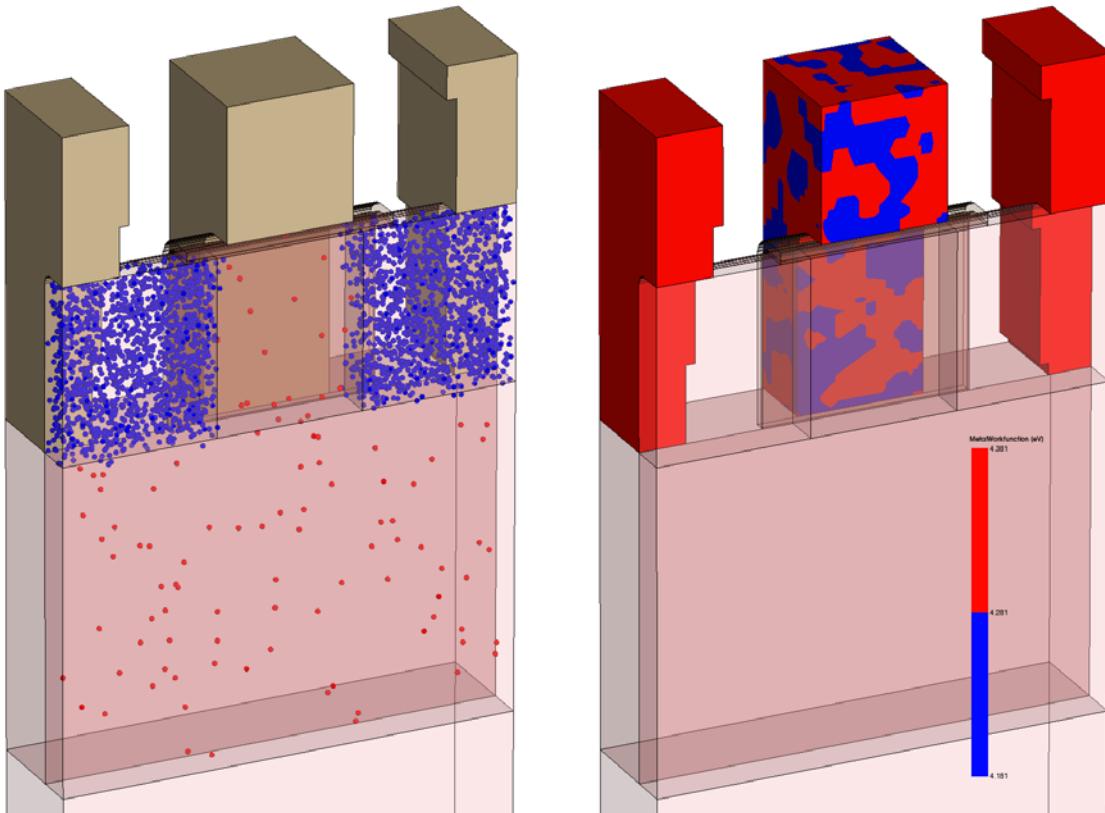
## Visualizing Variability Sources

This section discusses how different variability sources are visualized.

### Discrete Charges

The positions of discrete charges coming from random discrete dopants, interface-trapped charges (ITC), and user-added charges are written to the output TDR file as particle data (see [Table 10 on page 169](#)). This particle data can be visualized in Sentaurus Visual, as shown in [Figure 29 \(left\)](#).

**Figure 29** Visualization of statistical variability sources showing (left) random discrete dopants (donors in blue and acceptors in red) and (right) metal gate granularity showing the allocation of two different workfunctions to the metal grains



## Chapter 3: Simulation Setup

### Output

Table 10 Particle fields written by Garand

Discrete charge type	TDR particle field
RDD acceptors	Garand/Acceptors
RDD acceptor species	Garand/Acceptors/<species_field>
RDD donors	Garand/Donors
RDD donor species	Garand/Donors/<species_field>
ITC traps	Garand/Traps
SRH traps	Garand/TrapsSRH
User-added charges	Garand/AddedCharges

In Sentaurus Visual, the rendering options for particle data fields are available from the Region Properties dialog box (choose **Data > Region Properties**, and click the **Lines/Particles** button). Here, the shape and size used to render particles can be changed. The default sphere size used to render the particles can be set in the Sentaurus Visual preferences.

To change the sphere size:

1. In Sentaurus Visual, choose **Edit > User Preferences**.  
The User Preferences dialog box opens.
2. Expand **2D/3D > Plot**.
3. Under Particles, from the **Initial Sphere Size** list, select the value.
4. Click **Save**.

### Line Edge Roughness

Line edge roughness modifies the device structure. Therefore, any variation in the structure will be visible by looking at the TDR file in Sentaurus Visual.

## Chapter 3: Simulation Setup

### Output

#### Metal Gate Granularity

When metal gate granularity is activated in a simulation, additional fields are written to the TDR file:

- The `MetalGrains` field illustrates the generated metal grain pattern by assigning a value from 1 to  $n$  (where  $n$  is the number of grains) to each mesh node in the metal gate depending on which particular grain it is part of.
- The `MetalWorkfunction` field shows the actual workfunction assigned to each metal grain, as illustrated in [Figure 29 on page 168 \(right\)](#). Any values displayed outside of the metal gate are ignored.

#### Value Mapping in TDR Files

In TDR files, certain fields are represented by integers. The mapping used is specified here.

**Contacts** Shows the contact nodes and connected semiconductor regions

Mapping:

-1	Other	4	Gate Contact	12	Substrate Contact
0	Source Contact	8	Polysilicon	13	Drain Region
2	Source Region	11	Substrate Region	16	Drain Contact

---

#### Exporting 1D Cutline Data

You can export 1D cutline data from an arbitrary line through the simulation domain, which might be useful, for example, for plotting doping profiles (see [Exporting 1D Cutline Data on page 880](#)).

To export 1D cutline data, use the following command:

```
output cutline <x1>=<d1> <x2>=<d2> data=<string> file=<string>
```

where:

- $<x1>$  and  $<x2>$  are any two of  $x$ ,  $y$ , and  $z$ . You must choose the two directions that are normal to the direction of the cutline. For example, for a cutline in the  $x$ -direction,  $<x1>$  and  $<x2>$  must be  $y$  and  $z$ :

```
output cutline y=<d1> z=<d2> data=<string> file=<string>
```

These specify the location within the Garand simulation domain of the cutline in 3D space, with the position in the specified normal directions being given by the values  $<d1>$  and  $<d2>$ . If the location of the requested cutline does not lie on a mesh line in the simulation domain, then the values along the cutline are interpolated from the values at the surrounding mesh nodes.

## Chapter 3: Simulation Setup

### Output

- `data` sets the quantity to be output along the cutline (see [Exporting 1D Cutline Data on page 880](#)).
- `file` specifies the name of the file to which the cutline data is exported. You can include placeholders in the file name (see [Exporting 1D Cutline Data](#)).

Cutlines that are independent of applied bias voltages are written into the results directory specified by the `output directory=<string>` command. Any cutline outputs that depend on applied bias conditions are written into a directory named with the  $V_d$  and  $V_g$  bias conditions. Only cutlines relating to doping concentrations are bias voltage independent.

### Examples

Extract data for a cutline in the x-direction giving the donor concentration along the Si–oxide interface in the middle of the device:

```
output cutline y=0.0 z=0.0 data=DonorConcentration  
        file='cutline-x-donors.dat'
```

Extract data for a cutline in the vertical z-direction giving the potential down through the middle of the device, and label the file with the applied gate voltage:

```
output cutline x=0.0 y=0.0 data=ElectrostaticPotential  
        file='cutline-z-potential-Vg%VG%.dat'
```

Use the same cutline, but through the drain end of the device, and label the file with the experiment name:

```
output cutline x=50.0 y=0.0 data=ElectrostaticPotential  
        file='%EXPT%-drain-potential.dat'
```

---

## Autocutlines

When you use the `simulation autoslice=on` command to extract a slice automatically in a cross section at the middle of the gate, there is also an option to automatically generate cutlines of the majority carrier density vertically and horizontally, in appropriate locations for calibration of inversion layer charge (see [Automatically Slicing a Structure on page 84](#)).

Typically, you would use this when calibrating the density gradient parameters against Poisson–Schrödinger solutions. The output of autocutlines is activated automatically when using `autoslice=on`.

To deactivate this output, use the command:

```
output autocutlines=off
```

Examples of cutline locations automatically selected in a nanowire and a FinFET are shown in [Figure 30](#), where  $V$  indicates the vertical cutline and  $H$  indicates the lateral (horizontal) cutline. The vertical direction is selected based on the location of the substrate contact if it is present. If there is no substrate contact, then the vertical direction is selected as the

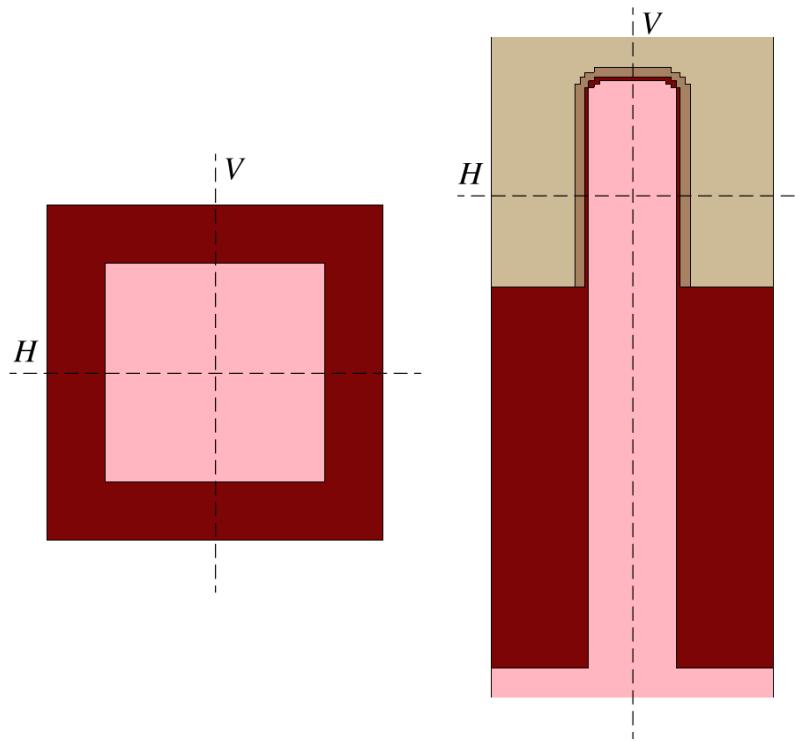
## Chapter 3: Simulation Setup

### Output

z-direction, unless the z-direction is the channel direction, in which case, the x-direction is used.

To decide on the location for the cutlines, Garand determines the extents of the semiconductor region that lies within the bounds of the gate and chooses the midpoint between those extents in either direction. In [Figure 30](#), for the nanowire, the cutlines are through the center of the wire in each direction. For the FinFET, the vertical cutline is down the center of the fin (assuming an entire FinFET is simulated), and the lateral cutline is halfway down the active part of the fin.

*Figure 30 Autocutline locations in (left) a nanowire and (right) a FinFET, where V indicates the vertical cutline and H indicates the horizontal cutline*



Garand writes to the screen the position and file names of each automatically generated cutline. If the automatically determined locations are not in the required position, then the position can be overridden in the input file.

To override the automatic position of the vertical cutline, use the command:

```
output vertical_autocutline_pos=<float>
```

where `<float>` is the absolute position (in input units) in the lateral direction at which the vertical cutline should be taken.

## Chapter 3: Simulation Setup

### Output

To override the automatic position of the lateral cutline, use the command:

```
output lateral_autocutline_pos=<float>
```

where `<float>` is the absolute position (in input units) in the vertical direction at which the lateral cutline should be taken.

Garand writes the generated cutlines into the bias-dependent output directory with a standardized naming convention:

- Vertical cutline: `auto-cutline-vertical-<carrier>.dat`
- Horizontal cutline: `auto-cutline-lateral-<carrier>.dat`

Here, `<carrier>` is either `eDensity` or `hDensity`, depending on the majority carrier type for the device being simulated.

---

## Extracting Integrated and Averaged Cutline Data

When comparing or calibrating to Monte Carlo simulations, it is useful to look at various integrated or averaged quantities from the drift-diffusion simulation along a cutline from the source end of the device to the drain.

### Integrated Charge Density

You can extract the carrier density (in  $\text{cm}^{-1}$ ), in cross sections across the device, integrated over the cross-sectional area to the file `integral_charge.dat` in the bias-dependent output directory.

To extract this quantity, use the input file command:

```
output integral_charge=on
```

### Weighted Average Velocity

You can extract the average velocity ( $\text{cm} \cdot \text{s}^{-1}$ ), in cross sections across the device, weighted by the carrier density, to the file `weighted_velocity.dat` in the bias-dependent output directory.

To extract this quantity, use the input file command:

```
output weighted_velocity=on
```

### Weighted Average Mobility

You can extract the average mobility (in  $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$ ), in cross sections across the device, weighted by the carrier density, to the file `weighted_mobility.dat` in the bias-dependent output directory.

## Chapter 3: Simulation Setup

### Output

To extract this quantity, use the input file command:

```
output weighted_mobility=on
```

## Limiting the Integration Range

You can limit the integration or averaging range to cover only a specific part of the device structure.

You set the limit of the integration range (in input units), in the considered direction, by using the following parameters:

```
output integration_xmin=<float>
output integration_xmax=<float>
output integration_ymin=<float>
output integration_ymax=<float>
output integration_zmin=<float>
output integration_zmax=<float>
```

You can also limit the integration to include only mesh elements that contain specific materials or that are part of specific regions. To limit to specific materials, use the command:

```
output integration_material=<string>
```

where `<string>` is a comma-separated list of materials.

To limit to specific regions, use the command:

```
output integration_region=<string>
```

where `<string>` is a comma-separated list of region names.

A mesh element is included in the integration if it meets the criterion of either list.

---

## Monte Carlo Transfer File

For details about Monte Carlo transfer (MCT) file output, see [Monte Carlo Transfer Files on page 48](#). This places several restrictions on the simulation type and models that can be applied.

To switch on MCT output, use the following input file command:

```
output mc_transfer=on
```

An `.mct` file is produced for every I–V point simulated. By default, the output MCT file is written into a subdirectory named `mct` within a directory named with the  $V_d$  and  $V_g$  bias conditions, unless the hierarchical output from Garand is switched off, in which case, the MCT file is written into the results directory. For details about the hierarchical input file option, see [Hierarchy of the Output Directory on page 188](#).

## Chapter 3: Simulation Setup

### References

The MCT file is named with the device number within the statistical ensemble (1 by default). For example:

```
<experiment>_1.mct
```

---

## References

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### References

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#### References

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## **Part II: Garand MC: Monte Carlo Simulator**

---

This part of the *Garand User Guide* contains the following chapters:

- [Chapter 4, Introduction to Garand MC](#)
- [Chapter 5, Monte Carlo Input File](#)
- [Chapter 6, Output Visualization](#)
- [Chapter 7, Monte Carlo Simulation Models](#)

# 4

## Introduction to Garand MC

---

*This chapter introduces the Garand MC device simulator.*

---

### Functionality of Garand MC and Workflow

Garand MC is a three-dimensional, self-consistent, ensemble quantum-corrected Monte Carlo solver, capable of both electron and hole transport in various default calibrated materials.

The solution from Monte Carlo simulation is provided through the collection of statistical data taken directly, or indirectly, from particle distributions representing the electron or hole carrier distributions within the simulation domain. The particle distribution evolves during the simulation by the repeated application of periods of deterministic free flight and instantaneous stochastic scattering events. Carriers move through the real-space simulation domain during free flight and, given a local field, accelerate, while scattering, given a list of mechanisms, instantaneously affects the momentum of the carrier.

Within ensemble Monte Carlo, a carrier distribution is represented by an ensemble of simulation particles. This allows the calculation of statistical properties over the simulated particle distribution. Self-consistency is provided by solving the Poisson equation at regular intervals to obtain the electrostatic potential consistent with the simulated particle distribution. This then determines the field under which particles accelerate during free flight until the next Poisson solution. As the simulated particle ensemble evolves explicitly over time, evaluation of transient phenomena can be observed. Since the simulated particle ensemble is known at discrete points in time, carrier-carrier interactions can be included directly. This avoids the problem of describing carrier-carrier interactions stochastically, which requires assumptions to be made about the carrier distribution.

[Figure 31](#) shows how Garand MC fits into the workflow. It takes as input a solution from a Garand simulation or, optionally, the solution from an earlier Monte Carlo simulation. The input to Garand MC completely specifies the simulation domain, its boundary conditions, and the initial state.

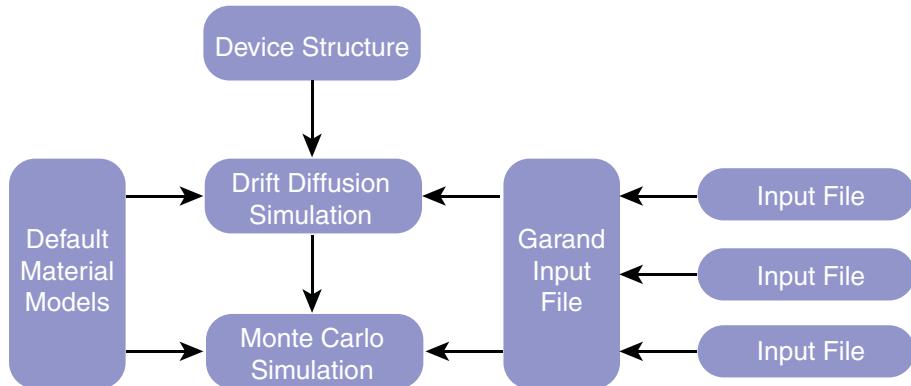
Default material models are defined equivalently for Garand and Garand MC, and are inputs to both. You can define nondefault material models by modifying the default parameters using input file commands.

## Chapter 4: Introduction to Garand MC

### Solution Approaches

One common input file is parsed by both Garand and Garand MC. The input file, however, can be split over multiple separate files that are read as one file using `import` commands. This allows for the convenient separation of commonly associated parameters or parameter sets for easy reuse, such as a particular mobility model calibration.

Figure 31 Flow diagram showing the relationship between the Garand simulator and the Garand MC simulator



---

## Solution Approaches

There are different ways in which you can run Garand MC, and all approaches converge on the device current as the main result:

- *Self-consistent ensemble MC* propagates an ensemble of carriers in time, while continuously solving the electrostatic potential. As such, carriers interact with each other and the solution recovers the transient behavior of the ensemble as it reaches steady state. The time-averaged potential, as well as carrier distribution, is obtained (see [Self-Consistent Ensemble Simulation on page 192](#)).
- *Single-particle MC* propagates an ensemble of carriers but in a fixed potential. As such, carriers do not interact, and the ensemble realizes a set of single-particle simulations running in parallel. Carriers sample the steady state only and transient behavior cannot be observed. The steady-state carrier distribution and current are obtained (see [Single-Particle Simulation on page 193](#)).
- *Backward MC* propagates a limited set of carriers from the virtual source back to the device contacts, where the probability of the corresponding forward trajectory is determined. Given a statistical sample of such trajectories, the device current can be determined. As with frozen field, the trajectories are through a fixed electrostatic potential and are independent of each other. As the set of trajectories is typically too small to sample the domain, only the steady-state current is obtained (see [Backward Monte Carlo Simulation on page 193](#)).

## Chapter 4: Introduction to Garand MC

### Solution Approaches

Results of frozen-field and backward MC simulations are seen to depend on the electrostatic potential used. If simply read from some other solution, such as drift diffusion, there is no guarantee that the potential is self-consistent with the MC carrier transport. Therefore, by default, all simulations start with a self-consistent ensemble MC period during which the carrier distribution and potential are allowed to reach steady state before one of the solution approaches is used to determine the current.

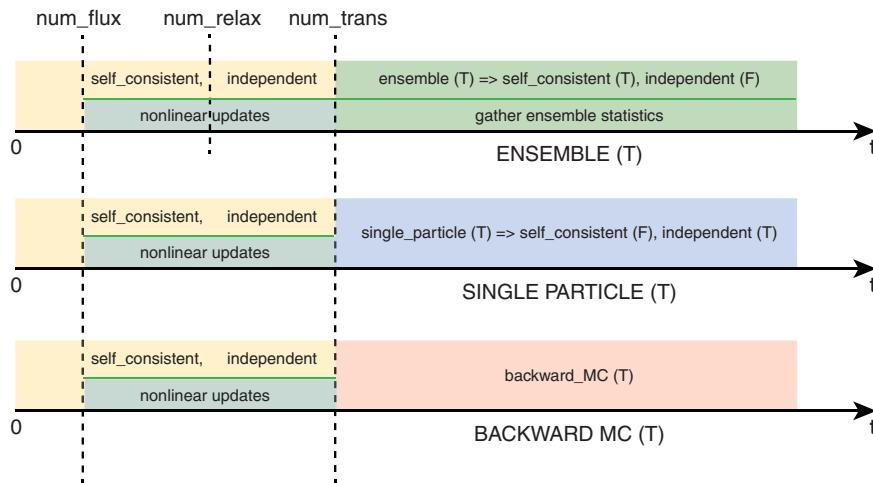
This initial self-consistent period can be removed by asserting a frozen-field simulation.

The different simulation approaches, together with the effect of asserting frozen field at the start of the simulation, are highlighted in [Figure 32](#) (see [simulation Command on page 884](#)).

**Figure 32** *Different simulation approaches*

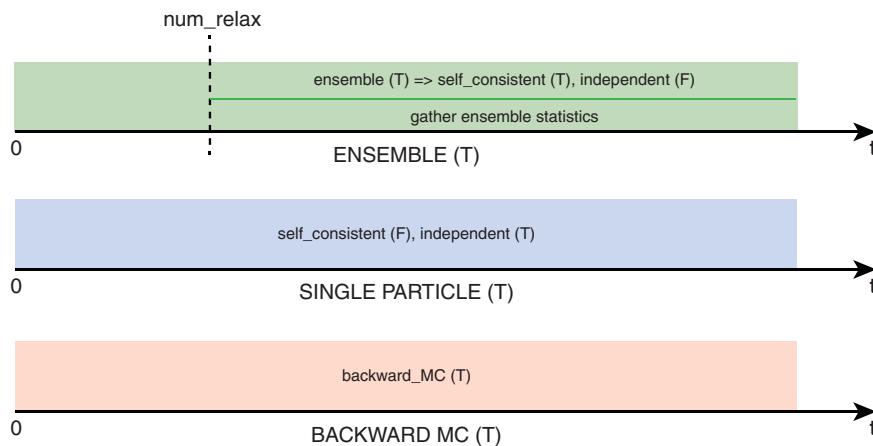
#### FROZEN\_FIELD (F)

At the end of transient, charge, potential, ensemble energy, and momentum are at steady state.



#### FROZEN\_FIELD (T) => self\_consistent (F), num\_flux (0), num\_trans (0)

At start of simulation, charge and potential are at steady state. Ensemble energy and momentum must relax.



## Particle Propagation

This section discusses particle propagation.

---

### Particle Ensembles

A particle ensemble represents the carrier distribution under investigation within the simulation domain and consists of a collection of simulation particles, with the state of each particle given at discrete points in time over the course of a simulation. A simulation can consist of both electron and hole particle ensembles for simulation using Garand MC.

Carrier distributions can be defined by particle ensembles in which individual carriers are represented by individual particles. In such cases, carrier-carrier interactions are resolved within the classical limit. Alternatively, you can define carrier distributions as fixed-size particle ensembles. In this case, each particle represents a collection or fraction of electrons, dependent on the total carrier charge within the simulation domain. For example, the simulation of nanoscale devices with large fixed ensemble sizes typically results in more particles than free electrons, and each particle within the ensemble represents a fraction of an electron. In such cases, short-range carrier-carrier interactions are removed and replaced progressively by an averaged interaction.

---

### Electron Transport

Electron transport within the conduction band is described by the propagation of carriers in an analytic multivalley band model, subject to intravalley and intervalley scattering. The number of valleys and their properties depend on the material model, with default definitions provided for a number of materials. In addition, each valley has a number of scattering mechanisms that apply to carriers associated with it and, again, default definitions are provided for each material valley model.

---

### Hole Transport

Hole transport within the valence band is described by the propagation of carriers in a six-band  $k \cdot p$  band structure. This leads to three bands in which, analogously to the valley model within the conduction band, each band has an associated set of intraband and interband scattering mechanisms. These models are defined by default for each material model.

Alternatively, hole transport can be described using the same analytic multivalley approach as used for electrons. This reduces the computational overhead associated with the six-band  $k \cdot p$  model, but at the cost of physical accuracy.

## **Self-Consistency**

Monte Carlo simulations can be performed self-consistently, meaning that the electrostatic potential that drives the carrier distribution is itself the solution of the charge distribution of the carrier (including external applied biases and variation in permittivity throughout the simulation domain).

In self-consistent simulations, particle distributions interact with themselves over long ranges through the self-consistent mesh-resolved potential. Short-range particle-particle interactions can be partially resolved in the same way, depending on the size of the mesh spacing.

---

## **Linear Poisson Solution**

The self-consistent potential is obtained from the solution of the Poisson equation, given the net charge assigned to the simulation mesh. The charge accounts for the fixed donor and acceptor doping, the fixed continuous carrier distributions (those not being solved by Monte Carlo particle propagation), and the Monte Carlo particle ensembles. The Poisson equation is solved at regular time intervals defined by the field-adjusting time step. Particle propagation over this time step is limited to a single evaluation of the field, so as to remove possible artificial heating associated with particle self-interactions. The field-adjusting time step is then the limiting factor affecting the accuracy in resolving particle dynamics.

---

## **Nonlinear Poisson Solution**

As part of a self-consistent simulation, the nonlinear Poisson solution is performed intermittently to re-solve continuous carrier concentrations through the simulation domain. This is required to allow the otherwise fixed continuous carrier distributions to respond to variations in the average particle distributions. The frequency of this nonlinear update is controlled by the value of the parameter `num_nlin` (see [Nonlinear Time Steps on page 196](#)).

---

## **Frozen-Field Approximation**

If self-consistency is not required, a Monte Carlo simulation can proceed using only the initial electrostatic potential solution from a drift-diffusion simulation. In this case, the carrier distribution is not coupled to the potential. Therefore, carrier-carrier interactions, at any range, are no longer resolved dynamically. The simulation proceeds as a series of parallel one-particle Monte Carlo simulations, one for each particle within the simulation domain. The nonlinear update to the potential and fixed carrier concentration still occur, providing some measure of self-consistency (see [Nonlinear Poisson Solution](#)).

## Quantum Corrections

Quantum corrections can be applied within Monte Carlo simulations analogously to their application within drift-diffusion simulations. Quantum correction is applied by the density gradient or 2D Poisson–Schrödinger effective quantum potential. This is obtained as a correction to the classical potential given the classical and effective quantum potentials from a drift-diffusion solution. The correction is fixed throughout a Monte Carlo simulation and is applied to the self-consistent electrostatic potential to obtain a time-varying effective quantum potential. This quantum potential then defines the driving force that determines particle propagation.

---

## Fermi–Dirac Statistics

In highly doped semiconductors or those with a low effective mass and correspondingly low density-of-states, degenerate statistics might be required. This manifests itself in drift-diffusion and Monte Carlo simulations through the equilibrium carrier statistics, and in Monte Carlo particle propagation by the rejection of scattering events based on the occupation probability of the final state. For more information about applying Fermi–Dirac statistics, see [Fermi–Dirac Carrier Statistics on page 130](#).

---

## Gathering Statistics

Garand MC assumes that device terminal currents are the intended outcome from all simulations. Results of terminal current estimation are written to screen and an output file, along with some other information that is useful for diagnostic purposes.

---

## Ramo–Shockley Estimation of Terminal Currents

Terminal currents are estimated using the Ramo–Shockley theorem, whereby the motion of all particles within the simulation domain, at a point in time, contribute to the terminal currents at that time for all terminals. Within this model, displacement currents are resolved and affect terminal currents during transient periods. Currents are estimated at the end of each field-adjusting time step and are based on the particle distribution at that time point.

---

## Estimation of Charge Flux Current

In addition to the Ramo–Shockley estimation of terminal currents, estimation is provided by defining local time derivatives of the net charge flux across terminal boundaries due to particle propagation. This model does not account for displacement currents but results in

---

the same steady-state current as estimated by Ramo–Shockley. Currents are estimated at the end of each field-adjusting time step and are based on the net flux of particles over the terminal boundaries during the time step.

---

## Estimation of Integrated Current Density

Another current estimation is provided by integrating the current density over a user-defined volume within the simulation domain. The integrated current density, charge flux, and Ramo–Shockley estimations should all converge in the steady-state regime.

---

## Estimation of Current Error

Uncertainty in the terminal current estimation is provided by the standard deviation of the current, given datasets composed of terminal currents defined at all previous time steps (omitting a defined transient period). Uncertainties are estimated in this way for both Ramo–Shockley and charge flux models. In both cases, independent samples are obtained by estimating the correlation length of the current–time signal.

Since Ramo–Shockley current estimations depend on the summation over carrier velocities, the correlation of the estimated current with time is linked to the carrier momentum relaxation times. However, charge flux estimates are based on the (almost) independent arrival of carriers at a point. Statistical uncertainty of the two estimators is therefore similar, despite the apparent same large size for Ramo–Shockley estimations.

---

## Scattering Statistics

During Monte Carlo simulations, incidences of carrier-scattering events associated with the included mechanisms are recorded. This information is presented at regular intervals throughout simulations.

---

## Carrier Statistics

Monte Carlo simulations gather information about carrier distribution throughout the simulation domain. Ensemble average carrier densities, energies, velocities, and current densities can be output optionally.

# 5

## Monte Carlo Input File

---

*This chapter describes the syntax and parameters of the input file for Garand MC. The input file controls execution of the simulation and allows some flexibility over simulation output.*

---

### Starting Garand MC From the Command Line

Before running a Monte Carlo (MC) simulation, you must run a drift-diffusion simulation of the structure at the required bias. This defines the simulation domain and provides the initial state for the MC simulation.

Garand MC receives this information in a Monte Carlo transfer (MCT) file, which is produced from a drift-diffusion simulation when the following command is specified:

```
output mc_transfer = on
```

For information about running Garand with this parameter, see [Monte Carlo Transfer Files on page 48](#).

The MCT file has the extension `.mct` and, by default, is placed in the `mct` directory at the same level as the `viz` directory, as specified in [Monte Carlo Transfer File on page 174](#). For example, if no substrate bias is specified in the input file, then the directory structure is as follows:

```
<directory>/Vd<drain_bias>_Vg<gate_bias>/mct/  
<experiment>_<device_number>.mct
```

If a substrate bias is defined, then the directory is extended to:

```
<directory>/Vd<drain_bias>_Vg<gate_bias>_Vsub<substrate_bias>/
```

Alternatively, if hierarchical output is deactivated in Garand, then the `.mct` file is written directly into the output directory:

```
<directory>/<experiment>_<device_number>.mct
```

See [Hierarchy of the Output Directory on page 188](#).

## Chapter 5: Monte Carlo Input File

### Starting Garand MC From the Command Line

Then, you run Garand MC by using the following command for a given bias condition:

```
garand-mc -fdd <path_to_mct_file> -f <path_to_input_file>
```

You can also define the MCT file in the input file by using the command:

```
structure mct_file = <path_to_mct_file>
```

This modifies the command to:

```
garand-mc -f <path_to_input_file>
```

The input file must then differ for each bias condition, which can be achieved using parameter substitution with Sentaurus Workbench, for example.

Command-line options control certain aspects of the simulation, allowing you to override specifications in the input file as required.

*Table 11 Command-line options for Garand MC*

Option	Description
-f <string>	Mandatory. Sets the name of the input file. Include the path if the file is not in the current working directory.
-b   --bands	Writes k·p band structure and terminates the simulator.
-c   --compatible <string>	Loads any available material files to align to a different tool or previous version (see <a href="#">Parameter Compatibility on page 191</a> ). It also can load any available parameter set for tabulated bands (see <a href="#">Full Band Model on page 284</a> ) by specifying: -c tabulated
-fdd <string>	Loads an MCT file. Include the path if the file is not in the current working directory.
-h   --help	Prints help message and exits.
--max_threads <integer>	Sets the maximum number of parallel threads to use when running Garand on a multicore system (see <a href="#">Parallel Execution on page 41</a> ).
--threads <integer>	Sets the number of parallel threads to use when running Garand on a multicore system (see <a href="#">Parallel Execution</a> ).
--verbose	Generates verbose screen output.

## Parallel Execution

To set up parallelization for Garand MC, see [Parallel Execution on page 41](#).

---

## Setting Up an Input File

The Garand MC input file includes the following commands:

- `simulation` commands define the execution of the MC simulation. They control, among other things, the number and the length of the simulation time steps, the carrier species to propagate, the number of particles, and whether or not the simulation is self-consistent with the potential.
  - `material` commands allow you to define nondefault material models and parameter values.
  - `output` commands define which fields, such as potential and material, are included in output TDR files for visualization.
- 

## Comments and Space

Space is ignored at the start of a line in the input file, and multiple spaces between parameters are treated as one space. When writing an input file, you can ignore space to allow for clearer formatting.

You can add comments in the input file. A comment can extend over one line if the first nonblank character is a hash character (#). Inline comments can be included after a complete command, at the end of a line, using the hash character.

---

## Hierarchy of the Output Directory

Results of a MC simulation are written to a directory specified in the input file by using:

```
output directory = <path_to_folder>
```

This directory can be the same for both the initial Garand and subsequent Garand MC simulations, or they can differ.

You control the depth of the hierarchy by using the following command:

```
output hierarchical=on
```

The default is `hierarchical=on`.

## Chapter 5: Monte Carlo Input File

### Hierarchy of the Output Directory

For example, after an initial drift-diffusion simulation for an  $I_d$ - $V_g$  curve, the following directory structure is created:

```
<directory>
|—— Vd<drainBias>_Vg<gateBias>[_Vsub<substrateBias>]
|   |—— <exp>_IdVg_Vd<drainBias>[_Vsub<substrateBias>]_<deviceNumber>.dat
|   |—— mct
|   |   |—— <exp>_<deviceNumber>.mct
|   |   |—— ...
|   |   |—— ...
|   |—— viz
|   |   |—— <exp>_<deviceNumber>.tdr
|   |   |—— ...
|   |   |—— ...
|—— ...
```

After the MC simulation, directories are created where results from the simulation are written, creating the following directory structure:

```
<directory>
|—— Vd<drain_bias>_Vg<gateBias>[_Vsub<substrateBias>]
|   |—— <experiment>
|   |   |—— data
|   |   |   |—— ...
|   |   |   |—— ...
|   |   |—— rates
|   |   |   |—— ...
|   |   |   |—— ...
|—— viz
|   |—— <experiment>-MC-Input.tdr
|   |—— <experiment>-MC-Output.tdr
|   |—— ...
|—— ...
```

Where the specified output directory is the same for both drift-diffusion and MC simulations, the results are at the same level, sharing the same `viz` directory.

#### Note:

A directory named by the simulation experiment name is created to store data associated with the MC simulation.

If you set `output hierarchical=off`, then all output data is written to the results directory, so the output after the drift-diffusion simulation is now:

```
<directory>
|—— <exp>_IdVg_Vd<drainBias>[_Vsub<substrateBias>]_<deviceNumber>.dat
|—— <exp>_<deviceNumber>.mct
|—— <exp>_<deviceNumber>.tdr
|—— ...
```

## Chapter 5: Monte Carlo Input File

### Simulation Parameters

After the MC simulation, the `data` and `rates` directories are retained:

```
<directory>
|__ Vd<drainBias>_Vg<gateBias>[_Vsub<substrateBias>]
|__ data
|   |__ ...
|   |__ ...
|__ rates
|   |__ ...
|   |__ ...
|__ <experiment>-MC-Input.tdr
|__ <experiment>-MC-Output.tdr
|__ ...
```

#### Note:

It is recommended that you set `output hierarchical=off` in Garand when using Sentaurus Workbench in hierarchical mode.

---

## Intermittent Output Files

In the `data` and `experiment` directories, Garand MC writes a file giving an overview of the results of the MC simulation, with current, velocity, energy, and band occupations, and a summary of scattering events. Separate files for electron and hole transport are created named `INTERMITTENT_ELEC_OUTPUT` and `INTERMITTENT_HOLE_OUTPUT`, respectively.

---

## Simulation Parameters

The nature of a MC simulation is determined by a set of parameters that define the following:

- Whether electron or hole particle transport is considered
- Whether the simulation is performed with a self-consistent potential
- Length of the field-adjusting time step
- Length of an initial transient period
- Maximum number of time steps the simulation should run for
- Current convergence criteria

All simulation parameters are specified in the input file using the following syntax (see [simulation Command on page 884](#)):

```
simulation <parameter>=<value>
```

## Parameter Compatibility

The `--compatible` command-line option allows you to choose between nondefault parameter sets if they exist. Such parameter sets might provide backward compatibility with previous versions or compatibility with other tools whose default parameter sets differ.

The option takes a string that is prepended to installed material parameter files. By convention, the string is the version number or the name of a tool for which a compatible parameter set has been provided. For example, with the following command, Garand MC attempts to read default material files starting with `sband`:

```
garand-mc -f <path_to_input_file> -fdd <path_to_mct_file>
--compatible sband
```

This will match the default silicon definition file `sband_Silicon.mat`, in which the material parameters and models have been defined consistently with Sentaurus Band Structure (`sband`). If no match is found, then the default material definition is used.

Compatible parameter sets are provided for the following:

- `sband_Silicon.mat`
- `O-2018.06_Silicon.mat`
- `O-2018.06_Germanium.mat`
- `O-2018.06_SiliconGermanium.mat`
- `O-2018.06_SiGe10.mat`
- `O-2018.06_SiGe20.mat`
- `O-2018.06_SiGe30.mat`
- `O-2018.06_SiGe40.mat`
- `O-2018.06_SiGe50.mat`
- `O-2018.06_SiGe60.mat`
- `O-2018.06_SiGe70.mat`
- `O-2018.06_SiGe80.mat`
- `O-2018.06_SiGe90.mat`
- `Q-2019.12_Silicon.mat`
- `Q-2019.12_Germanium.mat`
- `Q-2019.12_SiliconGermanium.mat`

## Chapter 5: Monte Carlo Input File

### Simulation Parameters

- tabulated\_GaN.mat
- tabulated\_Silicon.mat
- tabulated\_Germanium.mat
- tabulated\_SiliconGermanium.mat

#### Note:

To use the O-2018.06 parameters, you might need to include backward compatibility options for scattering (see [Backward Compatibility: Hole Scattering on page 353](#)).

---

## Electron and Hole Transport

Given a simulation domain solution from an earlier drift-diffusion simulation, both electron and hole carrier densities are defined. Either species can be resolved as particles and simulated using Garand MC, regardless of the majority carrier type.

The `electrons` and `holes` parameters define whether the associated carrier distributions are subject to a MC simulation. By default, electrons and holes are not specified for MC simulations. However, as a minimum requirement, you must specify one carrier type (see [simulation Command on page 884](#)).

#### Example

Specify that both electrons and holes are resolved as particles and propagated in the simulation:

```
simulation electrons=on  
simulation holes=on
```

---

## Self-Consistent Ensemble Simulation

Given the solution from an earlier drift-diffusion simulation, the equilibrium electrostatic potential is defined. You can perform a self-consistent ensemble MC simulation in which the electrostatic potential is reevaluated at the end of each field-adjusting time step.

The `ensemble` parameter defines whether to perform a self-consistent ensemble simulation (see [simulation Command on page 884](#)).

#### Example

Specify that an ensemble MC simulation proceeds self-consistently:

```
simulation ensemble=on
```

## Single-Particle Simulation

Given the solution from an earlier drift-diffusion simulation, the equilibrium electrostatic potential is defined. You can perform a single-particle simulation under the *frozen-field approximation* in which the electrostatic potential is unchanged between field-adjusting time steps. The `single_particle` parameter defines whether carrier propagation is performed within the frozen-field approximation (see [simulation Command on page 884](#)).

### Example

Specify a single-particle MC simulation:

```
simulation single_particle=on
```

---

## Backward Monte Carlo Simulation

Given the solution from an earlier drift-diffusion simulation, the equilibrium electrostatic potential is defined. You can perform a backward MC simulation in which carrier trajectories are initialized over a plane at the virtual source and followed back to the device contacts [1]. Each trajectory samples the current, from which the mean and standard deviation of the distribution can be defined. Given sufficiently numerous samples, the relative error in the mean converges to within the current tolerance and the result is returned. During backward MC simulation, the electrostatic potential is fixed, and the current is a function of this potential.

The `backward_mc` parameter determines whether to perform a backward MC simulation (see [simulation Command on page 884](#)).

### Example

Specify a backward MC simulation:

```
simulation backward_mc=on
```

---

## Frozen Field Modifier

By default, the electrostatic potential at the start of a MC simulation is assumed to be inconsistent with the MC carrier transport. This might be true for a device simulation where the initial guess came from an uncalibrated drift-diffusion solution. It is generally necessary to allow this initial potential to relax, such that it is self-consistent with the transport. This occurs through self-consistent updates to the potential at each time step, as well as nonlinear updates to the potential and Fermi levels using average carrier distributions sampled over nonlinear intervals.

## Chapter 5: Monte Carlo Input File

### Simulation Parameters

For single-particle and backward MC simulations, this is limited to the transient period at the start of the simulation, controlled by the number of transient time steps `num_trans`. In all cases covering ensemble, single-particle, and backward MC simulation solutions, the steady-state statistics are gathered after the transient period.

The `frozen_field` parameter is used to enforce that the initial transient is not required. This might be true for bulk simulations, for example, where the field is simply constant.

#### Example

Specify that the initial potential should be used without modification for the MC solution:

```
simulation frozen_field=on
```

---

## Field-Adjusting Time Step

The field-adjusting time step defines the period over which particles propagate assuming a constant field. At the end of this time step, electric fields are interpolated at the new positions of the particle, such that propagation proceeds during the next time step with an updated field.

If the simulation is self-consistent (see [Self-Consistent Ensemble Simulation on page 192](#)), then the electrostatic potential is re-solved based on the particle distribution at the end of the field-adjusting time step and before the field interpolation.

See [simulation Command on page 884](#).

#### Example

Specify a field-adjusting time step of 1 fs:

```
simulation DT = 1.0e-15
```

---

## Simulation Time Steps

You can specify MC simulations to run for a fixed time. This time is the length of the field-adjusting time step multiplied by a maximum number of time steps, and it is set by using the `num_steps` parameter (see [simulation Command on page 884](#)).

Depending on the details of the simulation and the measurement under investigation, a longer run might be required so that enough statistical information is gathered to limit the statistical error on any measurement to within some required bounds.

## Chapter 5: Monte Carlo Input File

### Simulation Parameters

#### Example

Specify a simulation consisting of 5000 time steps:

```
simulation num_steps=5000
```

---

## Charge-Flux Time Steps

The initial drift-diffusion solution defines a total carrier charge on which the MC particle charge is based. However, in general, the drift-diffusion solution and the total carrier charge do not match the MC solution. Self-consistent simulation allows excess charge to be removed from the contacts while a deficit charge is injected. An initial period of flux is assigned to allow this to occur and is defined by the `num_flux` parameter, which defines the number of time steps at the start of the simulation (see [simulation Command on page 884](#)).

The default number of time steps together with the default propagation time step yields a default flux period of 0.5 ps. Within this period, the linear Poisson solution is solved at the end of each propagation time step as in a self-consistent ensemble simulation. No nonlinear solutions are solved as the charge is expected not to be in equilibrium.

#### Example

Specify an initial flux period of 20000 time steps:

```
simulation num_flux = 20000
```

---

## Transient Time Steps

Given a solution from an earlier drift-diffusion simulation, both electron and hole carrier densities are defined.

A MC simulation initializes particles following this initial carrier distribution (see [Particle Initialization on page 253](#)), but it might be expected that differences in transport will lead to a slightly different equilibrium solution.

In addition, although particle positions are initialized following the initial solution, particle momenta are initialized assuming equilibrium and not considering the current density solution. Therefore, there is a transient period during which carriers reach an equilibrium. This transient period must be excluded, so that it does not contribute to the collection of steady-state statistics (see [simulation Command on page 884](#)).

#### Example

Specify an initial transient period of 75000 time steps:

```
simulation num_trans=75000
```

## Intermittent Time Steps

During MC simulations, at regular intervals, results are written to a file. This provides information about the progress of the simulation and convergence of statistical measures (see [simulation Command on page 884](#)).

### Example

Specify an intermittent period of 25000 time steps:

```
simulation num_inter=25000
```

---

## Statistics-Gathering Time Steps

The `num_stats` parameter takes a positive integer value and defines the number of time steps between which successive simulation statistics are gathered. The statistics-gathering time step captures ensemble carrier averages as a function of time as well as, following the transient period, position-dependent mesh averages and terminal currents as a function of time (see [simulation Command on page 884](#)).

For self-consistent device simulations, the required field-adjusting time step is so short (0.05 fs) that these statistics are highly correlated between successive time steps. Gathering statistics so frequently creates a significant simulation overhead with no benefit because only independent data samples can be used to reduce the statistical uncertainty in the result.

### Example

Specify that statistics are gathered every 100 time steps:

```
simulation num_stats=100
```

---

## Nonlinear Time Steps

In simulations where only one species of carrier is simulated by MC particle propagation, you must re-solve the continuous carrier concentration of the other species to retain self-consistency with the electrostatic potential, which in general will not be the same as the initial potential solution. This is achieved through the intermittent solution of the nonlinear Poisson equation, where continuous carrier concentrations are evaluated based on the potential and by using either Boltzmann or Fermi–Dirac statistics (see [Fermi–Dirac Carrier Statistics on page 130](#)).

See [simulation Command on page 884](#).

## Chapter 5: Monte Carlo Input File

### Simulation Parameters

#### Example

Specify an intermittent period of 1000 time steps:

```
simulation num_nlin=1000
```

---

## Superparticles

Given a simulation domain solution from an earlier drift-diffusion simulation and from which the continuous carrier distribution will be simulated by MC particle propagation (see [Electron and Hole Transport on page 192](#)), the number of particles used to resolve the continuous carrier distribution depends on whether particles will represent a single particle or are allowed to represent multiple or fractional charges.

The `superparticles` parameter defines whether particles resolving the initial continuous carrier distribution can have a nonunity electronic charge (see [simulation Command on page 884](#)).

By default, `superparticles=on` and the continuous carrier distribution can be represented by any number of particles, the number of electron particles being set by the `num_elec` parameter (see [Number of Electrons on page 199](#)). The total electron charge from the continuous distribution, together with the number of electron particles, determines the superparticle charge. The superparticle charge might be significantly less than 1 if a large number of particles is used to resolve a distribution in a small simulation domain.

If `superparticles=off`, particles are represented as individual carriers with unit electronic charge. The number of particles is fixed by the total charge from the initial continuous distribution (the number of particles fluctuates in the presence of Ohmic contacts and varies about the initial total charge if the initial solution is representative of the MC solution).

#### Example

Specify that the simulation treats the resolution of the initial continuous distribution as individual carriers:

```
simulation superparticles=off
```

---

## Monte Carlo Carrier Charge Reassignment

To reduce the accumulation of integration errors associated with large variation of charge and potential in regions of high charge density, you can apply a smoothing kernel repeatedly.

The kernel performs a cloud-in-cell reassignment of the MC-assigned charge distribution in regions of high density and, by reducing charge variation, it stabilizes self-consistent ensemble MC simulations.

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### Simulation Parameters

#### Note:

Iterating the charge reassignment multiple times reduces fluctuations in the charge density at the cost of spatial resolution and might impose an artificial distribution of charge.

#### Example

Switch off charge reassignment entirely by setting the number of iterations to zero (see [simulation Command on page 884](#)):

```
simulation iter_q_assign=0
```

---

## Tolerance

A MC simulation is assumed to solve for the drain terminal current and might exit early, before the specified number of simulation time steps is completed (see [Simulation Time Steps on page 194](#)), if the percentage error in the current estimate converges below a specified tolerance.

For low currents, where a small uncertainty in the current can represent a large percentage error, an alternate convergence test based on an absolute tolerance is performed.

See [simulation Command on page 884](#).

#### Example

Specify that the MC simulation will have converged when the error in the current is less than 3%:

```
simulation tolerance=3.0
```

Specify that the MC simulation will have converged when the uncertainty in the current is less than  $5 \times 10^{-9}$  A:

```
simulation abstol=5.0e-9
```

Deactivate this functionality:

```
simulation converge=off
```

In this case, the MC simulation will run for the total number of time steps.

#### Note:

Convergence of the current might occur quickly, especially for high current conditions. Convergence of position-dependent carrier distributions, such as average carrier density, energy, and velocity, might converge more slowly and depends on the number of simulated particles and the simulation mesh. If accuracy in mesh-dependent statistics is required, then either use a low value of

## Chapter 5: Monte Carlo Input File

### Simulation Parameters

the tolerance or deactivate convergence, in combination with a sufficiently large number of simulation time steps. Convergence on a mesh-dependent statistical property is not available.

---

## Number of Electrons

If you want to model electron transport using superparticles (see [Superparticles on page 197](#)), then you must specify the number of particles.

In small simulation domains, consistent with modern nanoscale devices, the default value of `num_elec` might result in a superparticle charge of less than unity (see [simulation Command on page 884](#)). In this case, the instantaneous discrete particle distribution represents a more continuous distribution. Direct short-range electron-electron interactions are reduced, and simulated dynamic screening is affected in this case.

Within a single-particle simulation, a self-consistent ensemble of particles can still be used during the initial period of charge flux. The size of the ensemble is specified by the `num_elec` parameter.

### Example

Set an initial number of 60000 electron particles:

```
simulation num_elec=60000
```

---

## Number of Holes

If you want to model hole transport using superparticles (see [Superparticles on page 197](#)), then you must specify the number of particles.

In small simulation domains, consistent with modern nanoscale devices, the default value of `num_hole` might result in a superparticle charge of less than unity (see [simulation Command on page 884](#)). In this case, the instantaneous discrete particle distribution represents a more continuous distribution. Direct short-range hole-hole interactions are reduced, and simulated dynamic screening is affected in this case.

Within a single-particle simulation, a self-consistent ensemble of particles can still be used during the initial period of charge flux. The size of the ensemble is specified by the `num_hole` parameter.

### Example

Set an initial number of 60000 hole particles:

```
simulation num_hole=60000
```

## Number of Independent Particles

It is only during the steady-state period, after the user-defined transient given by `num_trans`, that the difference between ensemble and single-particle MC simulation is seen.

The steady-state period is the period of statistics gathering that yields the MC solution. This is simulated as either a self-consistent ensemble or single-particle solution in a frozen field using an ensemble of independent particles.

If a single-particle simulation is defined (`single_particle=on`), then you must define the `num_elec_sp` and `num_hole_sp` parameters for electron transport and hole transport, respectively. This defines the number of independent particles to be used in the single-particle estimation of the steady-state solution (see [simulation Command on page 884](#)).

Within a single-particle simulation, the number of particles need not be one and can still be user-defined. Each particle is propagated independently throughout the domain as if running multiple single-particle simulations in parallel.

### Example

Set 5000 hole particles for steady-state single-particle simulation:

```
simulation num_hole_sp=5000
```

---

## Selection of Simulation Parameters and Troubleshooting

The default simulation parameters are suitable for typical silicon-based CMOS devices. However, for certain materials and device structures, you might need to modify them either to maintain numeric stability or to obtain certain outputs from a simulation.

*Table 12      Typical issues and solutions*

Issue	Feature	Actions
Degraded subthreshold slope	High source/drain doping	<ul style="list-style-type: none"><li>• Increase the number of particles (see <a href="#">Number of Particles</a>)</li><li>• Reduce mesh size (see <a href="#">Simulation Mesh</a>)</li><li>• Use single-particle simulation</li></ul>
	Light effective mass	<ul style="list-style-type: none"><li>• Reduce time step (see <a href="#">Time Steps</a>)</li></ul>

## Chapter 5: Monte Carlo Input File

### Selection of Simulation Parameters and Troubleshooting

Table 12    *Typical issues and solutions (Continued)*

Issue	Feature	Actions
Noise in output quantities (I–V, internal properties)	–	<ul style="list-style-type: none"><li>• Increase the number of particles (see <a href="#">Number of Particles</a>)</li><li>• Increase the number of time steps (see <a href="#">Time Steps</a>)</li><li>• Reduce convergence tolerance (see <a href="#">Convergence Criteria</a>)</li></ul>
Low field mobility lower or higher than expected	– Low-temperature simulation	<ul style="list-style-type: none"><li>• Check calibration of scattering mechanisms</li><li>• Increase transient period (see <a href="#">Time Steps</a>)</li><li>• Increase the number of time steps (see <a href="#">Time Steps</a>)</li><li>• Use a finer resolution of the scattering table (see <a href="#">Changing Default Parameter Values on page 339</a>)</li></ul>
Difference in electrostatics to reference simulation	–	<ul style="list-style-type: none"><li>• Check meshing (see <a href="#">Simulation Mesh</a>)</li></ul>

## Number of Particles

This section presents solutions to typical issues regarding the number of particles.

## Improving Stability

Where doping in the source and drain regions is high (for silicon, above  $2\text{e}20 \text{ cm}^{-3}$ ), simulations can be prone to numerical heating, which will present as a degradation in the subthreshold slope. This issue can be exacerbated by the inclusion of Fermi–Dirac statistics and the presence of quantum confinement in the source and drain regions (for example, in a nanowire transistor). This numerical heating is common in self-consistent particle simulations and, while it cannot be completely removed, it can be mitigated by the choice of simulation parameters.

Increasing the number of particles used in the simulation can improve stability, allowing smoother carrier and potential profiles and minimizing errors in the field. The introduction of Fermi–Dirac statistics influences this issue by distributing carriers to higher energies.

In general, using the default of 200 000 superparticles is reasonable (see [Superparticles on page 197](#)). However, increasing the value above 300 000 is often enough to resolve issues relating to numeric heating. In certain cases, it might be necessary to use a greater value (the maximum possible is 940 000), which will result in additional computational overhead,

## Chapter 5: Monte Carlo Input File

### Selection of Simulation Parameters and Troubleshooting

so immediately using the maximum value is not advisable where minimizing runtime is a consideration.

As previously noted, the main impact of this phenomenon is degradation in the subthreshold slope and, while this error is present above threshold, it is small enough to not strongly impact the drive current. Therefore, if the goal of the simulation is the on-current, it is reasonable to not mitigate this effect and ignore points in the subthreshold.

## Improving Convergence

Increasing the number of particles used in the simulation is also a way to improve convergence. This increases the number of trajectories simulated, which improves the sampling of real space and  $k$ -space, and reduces the uncertainty in the simulation output.

Again, this can degrade turnaround time, so use it with caution. While these values depend on the material and simulation domain, for state-of-the-art silicon-based devices simulating 300000 particles for 200000 time steps, this is a reasonable setup that should yield well-converged statistics.

---

## Time Steps

This section presents solutions to typical issues regarding time steps.

## Improving Stability

Reducing the propagation time step or increasing the simulation time can be used to offset errors present in the simulation.

Reducing the propagation time step (see [Field-Adjusting Time Step on page 194](#)) increases the integration accuracy and is particularly beneficial where the effective mass is low (typical of III–V materials or where stress has been applied) as the size of the change in momentum and energy due to the stochastic field error is inversely proportional to the effective mass. As this is another cause for numeric heating, the result is often degradation of the subthreshold slope.

Reducing the length of the time step necessitates an accompanying modification to the number of time steps to ensure the total simulation time is sufficient. An illustration of this is given in [Table 13](#). For self-consistent simulations, this results in an increased number of solutions of the Poisson equation, thereby increasing runtime.

However, as described in [Number of Particles on page 201](#), where the impact is in the subthreshold and the drive current is the main required outcome of the simulation, this change can be overlooked to maintain turnaround time.

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### Selection of Simulation Parameters and Troubleshooting

**Table 13** Number of time steps required for 10 ps simulation time with different propagation time step durations

Time step [s]	Value of num_steps
1e-17	1000000
2e-17	500000
3e-17	333334
4e-17	250000
5e-17 (default)	200000

The lighter mass can also influence the length of time required to reach steady state as the momentum relaxation time can increase; therefore, the length of the transient period should be extended (see [Transient Time Steps on page 195](#)). This might also be necessary in simulations where the ambient temperature is below 300 K. The default number of transient time steps is 40000, which is equivalent to 2 ps simulation time. The suitability of this can be assessed by examining the variation of energy over the simulation time (see [Time Evolution on page 247](#)) and ensuring steady state has been reached before the transient period ends.

## Improving Convergence

Increasing the total number time steps and, therefore, the total simulation time can be used to improve convergence in the same way as increasing the number of particles (see [Improving Convergence on page 202](#)). By default, a simulation terminates when either of the specified current convergence criteria have been met, so it might not run for the specified simulation time.

Therefore, it might be necessary to adjust or even deactivate the exit criteria to increase the number of trajectories, which would be useful where internal quantities (such as velocity, energy, or carrier distribution) are of interest, and these converge more slowly than current.

To deactivate exit on convergence, specify:

```
SIMULATION converge = off
```

Then, modify the number of time steps as necessary. For example:

```
SIMULATION num_steps = 200000
```

## Simulation Mesh

The simulation mesh can affect the stability, accuracy, and efficiency of the simulation, so care should be taken when setting it up.

Consideration should be given to preserving the thickness of each region or material so that, for example, the equivalent oxide thickness (EOT) is represented correctly. Take care to not create an unnecessarily fine or elongated mesh when trying to resolve the curvature.

Fine meshes introduce a computational overhead from the solution to the Poisson equation and can be detrimental to stability as a larger mesh spacing in regions of high density will reduce variations in charge, thereby minimizing accumulation of the stochastic impulse error.

A mesh spacing in the direction of the current flow of approximately 1 nm, while in the normal directions 0.25–0.5 nm should be sufficient to resolve the charge density with sufficient accuracy. In areas with low carrier density (for example, the substrate), mesh spacing can be large.

Where the symmetry of the device allows, the simulation of only half the structure can be used to reduce the size of the overall mesh. This can reduce the overhead introduced by the necessity of having a smaller mesh spacing. Care should be taken to ensure accuracy of results (see [External Boundaries on page 261](#)).

---

## Convergence Criteria

Noise in output quantities can be reduced by defining stricter convergence criteria. For high bias conditions, the current will converge relatively quickly, even with a low tolerance (1% or 2%). However, reducing the bias, in particular that applied to the gate, reduces the possibility of the current being defined with such certainty because fewer carriers access the channel. Therefore, in general, for gate voltages below the threshold, increase the tolerance and set `abs_tol` to a realistic value, consistent with the expected off-current for the given device.

Where a quantity other than current is the required outcome, for example, the velocity profile averaged along the channel or low field mobility, it might be preferable to deactivate the exit on convergence and to set the maximum number of time steps and carriers to sufficient values that will reduce the uncertainty in all gathered quantities. For details, see [Improving Stability on page 202](#) and [Improving Convergence on page 203](#).

For a full description of convergence criteria, see [Tolerance on page 198](#).

## Contact Parameters

Like Garand, you can control the behavior of contacts in MC simulations by using the `contact` command followed by one parameter per command line. For example:

```
contact <parameter>=<value>
```

---

### Decoupled Contacts

The injection and removal of carriers occurs at boundaries defined as Ohmic contacts. By default, these boundaries coincide with the fixed potential cell faces that define electrostatic contacts. You can change this default behavior to improve the stability and speed of the simulation by decoupling MC charge transport in a contiguous area around an electrostatic contact where carriers are in near-equilibrium and nonlocal transport is not important.

In this case, the initial drift-diffusion solution is a good approximation to the charge density within the decoupled region, and the injection or removal of carriers for MC transport simulation can be defined at the edge of the decoupled region. The decoupled contact region can be defined automatically or manually. For automatic definition, decoupled contact regions are defined around electrostatic contacts defined as the source and drain only when specified. The `decouple_source` and `decouple_drain` parameters control this behavior (see [contact Command on page 849](#)).

**Note:**

The default behavior is *not* to decouple contacts. Injection and removal of MC particles occurs at the boundary of electrostatic contacts.

**Example**

Decouple a region around electrostatic source contacts from MC transport automatically:

```
contact decouple_source=on
```

The automatically decoupled region is defined on a cell-by-cell basis where each decoupled cell must satisfy some criteria. Each decoupled cell must be adjacent to another decoupled cell or the electrostatic contact around which the region is being defined to create a contiguous region. Otherwise, a cell must satisfy one of the following constraints:

- [Decoupled Depth](#)
- [Decoupled Charge Difference](#)
- [Decoupled Field](#)
- [Decoupled Offset](#)

## Decoupled Depth

A cell is decoupled automatically if it is within a user-defined number of cells from an electrostatic contact specified by using the `decouple_depth` parameter (see [contact Command on page 849](#)).

### Example

Specify that a contiguous region four cells deep is defined automatically around source or drain contacts (subject to the value of `decouple_source` and `decouple_drain`):

```
contact decouple_depth=4
```

## Decoupled Charge Difference

A cell is decoupled automatically if the difference between the carrier density to be sampled with Garand MC and the net remaining charge density is less than a user-defined percentage specified by using the `decouple_diff` parameter (see [contact Command](#)).

### Example

Specify that cells in which the carrier density is within 0.2% of the remaining net charge density are included in an automatic definition of decoupled regions around source or drain contacts (subject to the value of `decouple_source` and `decouple_drain`):

```
contact decouple_diff=0.2
```

## Decoupled Field

A cell is decoupled automatically if the magnitude of the maximum field along any vertex is less than a user-defined value specified by using the `decouple_Emax` parameter (see [contact Command](#)).

### Example

Specify that cells in which the maximum field magnitude is less than 0.5 kV/cm are included in an automatic definition of decoupled regions around source or drain contacts (subject to the value of `decouple_source` and `decouple_drain`):

```
contact decouple_Emax=0.5
```

## Decoupled Offset

A cell is *not* decoupled automatically if the separation of the cell and the edge of a gate contact is less than a user-defined value specified by using the `decouple_offset` parameter (see [contact Command](#)).

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### Contact Parameters

#### Example

Specify that cells that are separated from a gate contact by more than 7 nm are included in an automatic definition of decoupled regions around source or drain contacts (subject to the value of `decouple_source` and `decouple_drain`):

```
contact decouple_offset=7.0
```

---

## Decoupled Regions

In addition to automatically defining decoupled regions around electrostatic contacts, you can specify decoupled regions generally by using the `structure` command with the following syntax:

```
structure decouple xmin | xmax | ymin | ymax | zmin | zmax = <float>
```

This command defines a bounding box within the simulation domain, inside of which the charge density is defined from the initial drift-diffusion solution and MC carriers are prohibited. MC carriers attempting to cross into the decoupled region are reflected.

If a user-defined decoupled region overlaps an electrostatic contact, then the decoupled region is treated as a decoupled contact, and the surface of the decoupled region defines Ohmic boundaries for the injection or removal of carriers.

If multiple regions overlap and one of the defined regions overlaps an electrostatic contact, then the surface of the union of overlapping regions defines Ohmic boundaries for the injection or removal of carriers.

#### Example

Define a bounding box with explicit limits in the x-direction, an explicit lower limit in the z-direction, and the y-direction defaults to the simulation domain limits:

```
structure decouple xmin = -10.0 xmax = 10.0 zmin = -50.5
```

---

## Velocity-Weighted Injection Distribution

Carriers injected at the contacts must be injected with a distribution characterized by an increased probability that high-velocity carriers within the equilibrium distribution cross the contact boundary. Such a distribution depends on the band structure and the statistical model, and the selection of state must be evaluated numerically.

The `injection_dist` parameter controls whether the velocity-weighted injection distribution is evaluated for use in defining injection states. The default (`injection_dist=off`) defines carriers with an equilibrium energy distribution and assets only that the carrier velocity is aligned to the injection direction (see [contact Command on](#)

## Chapter 5: Monte Carlo Input File

### Contact Parameters

[page 849](#)). This results in average energies lower than using the velocity-weighted injection distribution as there is no preference for higher velocities.

#### Example

Specify to apply the velocity-weighted injection distribution when injecting carriers at Ohmic contact boundaries:

```
contact injection_dist=on
```

---

## Contact Resistance

Contact resistance can be defined for Garand MC using the same commands as for Garand (see [Contact Resistance on page 132](#)). For lumped resistance ( $\Omega$ ):

```
CONTACT resistance_lumped = <float>
CONTACT resistance_lumped_source = <float>
CONTACT resistance_lumped_drain = <float>
```

For lumped resistivity ( $\Omega \text{ cm}^{-2}$ ):

```
CONTACT resistivity_lumped = <float>
CONTACT resistivity_lumped_source = <float>
CONTACT resistivity_lumped_drain = <float>
```

The lumped resistivity is translated to a lumped resistance in the same manner as described in [Lumped Resistivity on page 133](#).

With contact resistance defined in the command file, the simulation proceeds as follows:

1. A Garand MC simulation without contact resistance begins.
2. After the current has converged to the defined tolerance, the source and drain contact potentials are updated based on the value of the resistance and the average current at that point.
3. The Garand MC simulation restarts using these updated boundary conditions, with carrier states retained from before the update.
4. Steps 2 and 3 are repeated until the relative change in the average current between updates is below a defined tolerance. Then, the Garand MC simulation runs until either the convergence criteria (see [Tolerance on page 198](#)) are met or the maximum number of time steps is reached.

The contact potentials are updated when the relative change in current from one update to the next is within a defined range, the bounds of which can be defined using:

```
CONTACT resistance_convergence_min=<float>
CONTACT resistance_convergence_max=<float>
```

## Chapter 5: Monte Carlo Input File

### Contact Parameters

These bounds are applied in a similar way as described on [Specifying a Lumped Contact Resistance on page 132](#), although the default values for Garand MC differ from those used by Garand and are both set to the same value defined for convergence criteria (see [Tolerance on page 198](#)):

```
SIMULATION tolerance=<float>
```

The tolerance is defined as a percentage, so setting this to 1% will result in the bounds for the relative change in current being set to 0.01. If the Garand MC simulation has completed and the relative difference in current, with reference to the previous update, is still greater than the maximum-allowed level, then the contact potential is updated with a limit of  $V_d/2$ .

As the application of contact resistance in Garand MC requires additional simulations, the runtime will always be greater than a typical Garand MC simulation where only the intrinsic behavior is required (this is the first step in simulations where contact resistance is applied). In addition to the bounds previously defined, several other commands can be used to limit this increase in runtime and these are defined here.

By default, a Garand MC simulation will complete, either by satisfying convergence criteria or by reaching the maximum number of time steps before the contact potential is updated. You can adjust the convergence criteria required before the contact potential is updated by using:

```
CONTACT resistance_tolerance=<float>
```

Increasing this value above that used to define convergence for the Garand MC simulation can reduce the time between updates for the contact potential and might result in a reduction in the total turnaround time. However, care should be taken with this parameter as a well-converged simulation generally completes faster.

The total number of times the contact potential is updated can be limited to prevent excessive simulation time, by using:

```
CONTACT resistance_loops_max=<integer>
```

The default is 20 and, typically, most simulations require approximately five iterations.

It is assumed that, in the subthreshold, the low current has minimal impact on the boundary conditions. Therefore, to avoid long simulations for gate bias points in the subthreshold, the drain current is required to exceed a threshold before the contact potentials are updated. This can be set using the command:

```
CONTACT resistance_current_min=<float>
```

The default is 1e-7 A. The optimal value for a given simulation depends on the threshold voltage for the simulation in question and the magnitude of resistance applied.

The intermittent output files are updated during the course of a simulation (see [Intermittent Output Files on page 190](#)), and the current stage is written to files using the standard

## Chapter 5: Monte Carlo Input File

### Material Definitions

naming convention. At the end of each Garand MC stage, before the contact potential is updated, the final result for that stage is written to a file with the stage number appended.

The time evaluation of ensemble average carrier properties is written to one file for the entire simulation, capturing each change to the contact potential (see [Time Evolution on page 247](#)).

The output visualization TDR file is written only for the final result if the following command is set (see [Steady-State Fields on page 242](#)):

```
output MC_results = on
```

To view the output TDR file after each update to the contact potential, use the command:

```
output MC_results_all = on
```

The default is `off` for this command because it might consume a substantial amount of disk space. Therefore, it should be used with care.

When setting up a Garand MC simulation, there are two important requirements:

- The scaling factor for the output current must be set correctly to ensure the magnitude of the contact potential modification is correct (see [Scaling the Output Current on page 74](#)).
- The initial Garand drift-diffusion simulation must not include contact resistance. Setting contact resistance where a transfer file is to be written will result in the simulation exiting with an error. Therefore, any contact resistance required to be simulated in Garand MC should be defined in the Garand MC command file and not in the common base input file.

---

## Material Definitions

All *default materials* are described by a default definition with default parameter values. The material definition is the model used to describe the material (see Part IV). For insulators and metallic contacts, the definition is simply a bulk model constituting a list of appropriate bulk parameters.

For semiconductors and semiconductor contacts, however, the material definition requires additional conduction band and valence band models. These models are themselves defined by a list of valley models with an appropriate list of valley parameters.

For MC simulations, valley models have an additional definition requirement of a scattering mechanism model, which defines a list of mechanisms that are active within the particular valley. The mechanisms themselves can have a list of parameter values specific to the scattering process. The collection of valleys and mechanisms, each with their parameter values, constitutes the semiconductor material definition. Of course, you can change the default model for each of these components and their values in the input file.

This section discusses how to change material definitions.

## Band Model

Each default material defines a list of available valley definitions that can be included to define the conduction band and valence band models. For a list of available valley definitions for each material, see Part IV.

The default band model for a material can use all, or only a subset, of the available valley definitions.

You can specify nondefault band models in the input file by adding or removing an allowed valley from the current material definition.

## Adding a Valley Definition

To add a valley definition to a material definition, use the following syntax:

```
material <material>.〈bandcontainer〉.〈band〉.〈valley〉 ADD
```

The 〈valley〉 must be the name of an allowed valley definition for material <material>. Attempting to add an undefined valley generates an error.

### Example

Add the L1 valley and G-valley (representing one of the eight  $L$ -conduction valley models and the  $\Gamma$ -conduction valley model) of silicon in the material definition:

```
material Silicon.conduction.C1.L1 ADD  
material Silicon.conduction.C2.G ADD
```

## Removing a Valley Definition

To remove a valley definition from a material definition, use the following syntax:

```
material <material>.〈bandcontainer〉.〈band〉.〈valley〉 REMOVE
```

The 〈valley〉 must be the name of an allowed valley definition that is currently included as part of the material definition for material <material>. Attempting to delete a valley that is not part of the current material definition generates an error.

### Example

Remove the X1 valley (representing one of the six  $X$ -conduction valley models) of silicon from the material definition:

```
material Silicon.conduction.C1.X1 REMOVE
```

## Scattering Mechanism Model

Each default valley defines a list of available scattering mechanism definitions that can be included to define the valley model. For a list of available mechanism definitions for each valley, see Part IV.

The default mechanism model for a valley can use all, or only a subset, of the available scattering mechanism definitions.

You can specify nondefault mechanism models in the input file by adding or removing mechanisms from the current valley definition.

### Adding a Scattering Mechanism Definition

To add a mechanism definition to a valley definition, use the following syntax:

```
material <material>. <bandcontainer>. <band>. <valley>. <mechanism> ADD
```

The <mechanism> must be the name of an allowed mechanism definition consistent with the named valley and material.

#### Example

Add the Brooks–Herring model of ionized impurity scattering as a mechanism for carriers in the  $\Gamma$ -valley of InGaAs:

```
material InGaAs.conduction.C2.G.II ADD
```

### Removing a Scattering Mechanism Definition

To remove a mechanism definition from a valley definition, use the following syntax:

```
material <material>. <bandcontainer>. <band>. <valley>. <mechanism> REMOVE
```

The <mechanism> must be the name of an allowed mechanism definition consistent with the named valley and material.

#### Example

Remove Ridley's third-body exclusion model of ionized impurity scattering as a mechanism for carriers in the  $\Gamma$ -valley of InGaAs:

```
material InGaAs.conduction.C2.G.II REMOVE
```

---

## Filtering Scattering Mechanisms

You can filter a set of defined scattering mechanisms in all valleys associated with the conduction band or valence band of a semiconductor material by defining a list of filters, which is controlled by the `scattering` parameter.

The list of scattering filters can be set in the input file by using the following syntax:

```
material <material>. <bandcontainer>. scattering <string>
```

where `<material>` is a named material or region within the simulation domain, and `<string>` is a list of one or more options available in [Table 14](#).

**Note:**

You can apply multiple filters in succession, in the order they appear in the list.

*Table 14 Options for filters*

Parameter	Description	Default
scattering <string>	Sets a list of filters, separated by space. Options are: <ul style="list-style-type: none"><li>• +All: Include all defined scattering mechanisms.</li><li>• -All: Remove all defined scattering mechanisms.</li><li>• +Acoustic: Include all defined acoustic phonon scattering mechanisms.</li><li>• -Acoustic: Remove all defined acoustic phonon scattering mechanisms.</li><li>• Ballistic: Remove all defined scattering mechanisms (same as -All).</li><li>• +II: Include all defined ionized impurity scattering mechanisms.</li><li>• -II: Remove all defined ionized impurity scattering mechanisms.</li><li>• +ImpactI: Include all defined impact ionization scattering mechanisms.</li><li>• -ImpactI: Remove all defined impact ionization scattering mechanisms.</li><li>• +Optical: Include all defined optical phonon scattering mechanisms.</li><li>• -Optical: Remove all defined optical phonon scattering mechanisms.</li><li>• +Pop: Include all defined polar-optical phonon scattering mechanisms.</li><li>• -Pop: Remove all defined polar-optical phonon scattering mechanisms.</li><li>• +RC: Include all defined remote Coulomb scattering mechanisms.</li><li>• -RC: Remove all defined remote Coulomb scattering mechanisms.</li><li>• +SR: Include all defined surface roughness scattering mechanisms.</li><li>• -SR: Remove all defined surface roughness scattering mechanisms.</li></ul>	+All

## Chapter 5: Monte Carlo Input File

### Material Parameters

#### Examples

Remove all scattering mechanisms from the conduction band of silicon:

```
material Silicon.conduction.scattering -all
```

This is the same as specifying:

```
material Silicon.conduction.scattering ballistic
```

Include only ionized impurity scattering:

```
material Silicon.conduction.scattering -all +II
```

---

## Material Parameters

Given a material definition, which can be modified from its default definition by using input file commands (see Part IV), default material parameter values can be similarly modified. Following the definition of a material as consisting of a bulk model with optional valley and mechanism models, the specification of nondefault parameter values is split into specifying bulk, valley, and mechanism parameter values.

---

## Channel and Substrate Orientations

For semiconductor materials, you can specify a nondefault orientation of the crystal, with respect to the simulation domain, by supplying orthogonal orientations for the channel and the substrate, using the following syntax:

```
material <material>.crystal.<direction> <h k l>
```

where:

- <material> is the unique name identifying a region or semiconductor material definition.
- <direction> is *x*, *y*, or *z*, and defines the simulation domain axis along which the crystal is aligned.
- <*h k l*> denote the Miller indices that define a direction within the crystal lattice that is then aligned to be colinear with the simulation domain direction. Each Miller index has the general form:

```
[r]I1 [+|- I2]
```

The optional *r* indicates to take the square root of the first integer *I1* and, optionally, to add that value to or, to subtract that value from, the integer value *I2*. For default material orientations, see Part IV.

## Chapter 5: Monte Carlo Input File

### Material Parameters

#### Note:

Ensure that the specified orientations are orthogonal. Otherwise, the orientation specification will be invalid and Garand MC terminates.

The following commands change the default orientation of silicon substrate to (110) and the channel orientation to  $\langle \bar{1}1\sqrt{2} \rangle$ :

```
material Silicon.crystal.z 1 1 0
material Silicon.crystal.x -1 1 -r2
```

You also can specify explicitly all orientation directions. For example:

```
material Silicon.crystal.x 1 1 0
material Silicon.crystal.y -1 1 0
material Silicon.crystal.z 0 0 1
```

Care must be taken if all three axes are defined because a right-handed rule is used. Therefore, the following definition is *not* valid in Garand MC:

```
material Silicon.crystal.x 1 1 0
material Silicon.crystal.y 1 -1 0
material Silicon.crystal.z 0 0 1
```

This would be a left-handed orientation. In this case, you would see an error message with suggestions for changing the specified orientation to make it valid.

---

## Changing Default Parameter Values

To change the default parameter values for bulk material models in the input file, use the following syntax:

```
material <material>.<parameter> <value>
```

where:

- <material> is the unique name identifying a material definition.
- <parameter> is the name of a bulk material parameter.
- <value> is the new value of the parameter, specified in the expected type.

For a list of bulk material parameters and their units, see Part IV.

### Example

Change the default value of the static dielectric constant of SiO<sub>2</sub> and the electron affinity of germanium:

```
material Oxide.permittivity 1.0
material Germanium.affinity 12.0
```

## Valley Parameter Values

For semiconductor material definitions, to change the default valley parameter values in the input file, use the following syntax:

```
material <material>.<bandcontainer>.<band>.<valley>.<parameter> <value>
```

where:

- <material>, <bandcontainer>, <band>, and <valley> are unique names that identify a material, a band container, a band, and one of its valley definitions.
- <parameter> is the name of a valley model parameter.
- <value> is the new value of the parameter, specified in the expected type.

For a list of valley parameters and their units, see Part IV.

### Example

Change the default value of the valley energy minimum and the nonparabolicity of the X1 valley in silicon:

```
material Silicon.conduction.C1.X1.E      0.95
material Silicon.conduction.C1.X1.alpha  0.55
```

---

## Scattering Mechanism Parameter Values

For semiconductor material definitions, to change the default parameter values of a scattering mechanism in the input file, use the following syntax:

```
material
<material>.<bandcontainer>.<band>.<valley>.<mechanism>.<parameter>
<value>
```

where:

- <material>, <bandcontainer>, <band>, <valley>, and <mechanism> are unique names that identify a material, a band container, a band, one of its valley definitions, and a scattering mechanism definition within the valley.
- <parameter> is the name of a parameter of the scattering mechanism model.
- <value> is the new value of the parameter, specified in the expected type.

For a list of mechanism parameters and their units, see Part III.

### Example

Change the default energy and coupling constant of the g-type intervalley optical phonon scattering mechanism g1x2 of the X1 valley in silicon, where X2 is the final valley:

```
material Silicon.conduction.C1.X1.g1x2.E 3.1d-2
material Silicon.conduction.C1.X1.g1x2.cc 2.3d9
```

---

## Defining Interface Models

Material interfaces can define models that alter bulk scattering mechanisms or can define parameters used by scattering mechanisms, such as surface roughness or remote Coulomb.

You must **first** define an interface model before you can associate parameter values with it. To define an interface model, use the `define` command with the following general syntax:

```
define <material1>.<material2>.<interface> <interface_model>
```

where:

- `<material1>` and `<material2>` are unique names of materials, or regions, that form the interface.
- `<interface>` is a unique user-defined name that identifies the interface model.
- `<interface_model>` is a keyword that specifies the type of model to be defined. Options are:
  - `alloy_interface`: [Alloy Scattering Interface Model on page 219](#)
  - `phonon_interface`: [Acoustic Phonon Interface Model on page 220](#)
  - `rough_interface`: [Rough Interface Model on page 220](#)
  - `trap_exponential`: [Exponential Interface Trap Distribution on page 221](#)
  - `trap_gaussian`: [Gaussian Interface Trap Distribution on page 222](#)
  - `trap_level`: [Interface Trap Level Model on page 223](#)
  - `trap_table`: [Tabulated Interface Trap Distribution Model on page 223](#)
  - `trap_uniform`: [Uniform Interface Trap Distribution Model on page 224](#)

When defined, all interface models automatically define a set of parameters that can be assigned in the input file by using the `interface` command with the following general syntax:

```
interface <material1>.<material2>.<interface>.<parameter> <value>
```

## Chapter 5: Monte Carlo Input File

### Scattering Mechanism Parameter Values

where:

- <interface> is the name of a previously defined interface model between <material1> and <material2>.
- <parameter> is a parameter associated with the interface model.
- While the set of parameters differs for different models, [Table 15](#) lists the parameters common to all models, except where noted.

*Table 15 Parameters common to interface models*

Parameter	Description	Type	Default
carrier	<p>Specifies the carrier type to which the interface model is tied. This can be useful for calibration where different values might give better results for different carriers. Options are:</p> <ul style="list-style-type: none"><li>• electrons</li><li>• holes</li></ul> <p>This parameter is optional. If not set, then the interface model matches both carriers. If set, then the model matches only when the specified carrier is simulated.</p> <p>If multiple interface models of the same type are defined between the same two materials, then the model that explicitly matches the carrier being simulated takes priority.</p> <p>If an exact match is not found, then the general carrier-independent model is used.</p>	string	–
DLN	Sets the number of discrete levels over which the trap distribution is integrated. The energy levels span the valence band edge to the conduction band edge, separated into 13 steps by default.	integer	13

**Note:**

This parameter applies only to interface trap distribution models.

## Chapter 5: Monte Carlo Input File

### Scattering Mechanism Parameter Values

*Table 15 Parameters common to interface models (Continued)*

Parameter	Description	Type	Default
orient	<p>Sets the <math>\langle hkl \rangle</math> crystal orientation of the interface and ties an interface model to a specific orientation. This parameter is optional.</p> <p>If not set, then the interface model matches all interfaces between the two named materials in the simulation domain.</p> <p>If set, then the model only matches interfaces between the two named materials in the simulation domain with the same orientation.</p> <p>If multiple interface models of the same type are defined between the same two materials, then the model that explicitly matches an interface in the simulation domain takes priority.</p> <p>If an exact match is not found, then the general orientation-independent model is used.</p>	vector	–
type	<p>Mandatory. Specifies whether traps are donor like or acceptor like. If you do not specify this parameter, an error is generated. Options are:</p> <ul style="list-style-type: none"> <li>• acceptor</li> <li>• donor</li> <li>• eneutral</li> <li>• fixedcharge</li> <li>• hneutral</li> </ul> <p>Use <code>acceptor</code> or <code>eneutral</code> to define the trap level as acceptor like. Use <code>donor</code> or <code>hneutral</code> to define the trap level as donor like. In these cases, the occupation of traps is calculated by using the Fermi–Dirac occupation function.</p> <p>You can specify <code>fixedcharge</code>, in which traps are always occupied, with the sign of the trap density in subsequent models determining whether or not they are donor like or acceptor like.</p> <p><b>Note:</b></p> <p>This parameter applies only to interface trap distribution models.</p>	string	–

## Alloy Scattering Interface Model

An alloy scattering interface model allows parameters to modify the alloy scattering potential in the presence of an interface to be defined. You assign parameters in the input file by using the `interface` command. In addition to the common parameters (see [Table 15](#)), an `alloy_interface` model defines the parameter listed here.

## Chapter 5: Monte Carlo Input File

### Scattering Mechanism Parameter Values

Table 16 Parameter specific to alloy\_interface model

Parameter	Description	Type	Default	Unit
AllPot	Sets the alloy potential factor.	float	1.0	-

#### Example

Define an alloy scattering interface model named All\_110, between SiliconGermanium and Oxide, that halves the alloy scattering potential under the interface for a (110) surface for electron transport:

```
define      SiliconGermanium.Oxide.All_110 alloy_interface
interface   SiliconGermanium.Oxide.All_110.carrier electrons
interface   SiliconGermanium.Oxide.All_110.orient  1 1 0          # <hkl>
interface   SiliconGermanium.Oxide.All_110.AllPot  0.5
```

## Acoustic Phonon Interface Model

An acoustic phonon interface model allows parameters to modify acoustic phonon scattering in the presence of an interface to be defined. You assign parameters in the input file by using the `interface` command. In addition to the common parameters (see [Table 15](#)), a phonon\_interface model defines the parameter listed here.

Table 17 Parameter specific to phonon\_interface model

Parameter	Description	Type	Default	Unit
AcDef	Sets the acoustic deformation potential factor.	float	1.0	-

#### Example

Define an acoustic phonon interface model named Ac\_111, between SiliconGermanium and Oxide, that doubles the acoustic deformation potential under the interface for a (111) surface for hole transport:

```
define      SiliconGermanium.Oxide.Ac_111 phonon_interface
interface   SiliconGermanium.Oxide.Ac_111.carrier holes
interface   SiliconGermanium.Oxide.Ac_111.orient  1 1 1          # <hkl>
interface   SiliconGermanium.Oxide.Ac_111.AcDef  2.0
```

## Rough Interface Model

A rough interface model allows parameters associated with surface roughness to be defined. You assign parameters in the input file by using the `interface` command. In

## Chapter 5: Monte Carlo Input File

### Scattering Mechanism Parameter Values

In addition to the common parameters (see [Table 15](#)), a `rough_interface` model defines the parameters listed here.

*Table 18 Parameters specific to rough\_interface model*

Parameter	Description	Type	Default	Unit
L	Sets the correlation length.	float	0.0	nm
RMS	Sets the root mean square (RMS) amplitude.	float	0.0	nm

### Example

Define a rough interface model named `rough_001`, between Silicon and Oxide, and assign the RMS amplitude and correlation length for a (001) surface calibrated for electron transport:

```
define      Silicon.Oxide.rough_001 rough_interface
interface   Silicon.Oxide.rough_001.carrier electrons
interface   Silicon.Oxide.rough_001.orient 0 0 1          # <hkl>
interface   Silicon.Oxide.rough_001.RMS    1.2            # nm
interface   Silicon.Oxide.rough_001.L      2.0            # nm
```

## Exponential Interface Trap Distribution

An exponential interface trap distribution model allows the association of parameters that describe an exponential distribution of traps over an energy range at an interface. In addition to the common parameters (see [Table 15](#)), a `trap_exponential` model defines the parameters listed here.

*Table 19 Parameters specific to trap\_exponential model*

Parameter	Description	Type	Default	Unit
E0	Sets the energy of the midpoint of the energy distribution relative to the valence band edge.	float	0.0	eV
Es	Sets the width of the energy range over which the trap density is defined.	float	0.0	eV
N0	Sets the magnitude of the trap density, such that the density is $N(E) = N0 \exp\left(-\left \frac{E - E0}{Es}\right \right)$ .	float	0.0	$\text{cm}^{-2} \text{eV}^{-1}$

## Chapter 5: Monte Carlo Input File

### Scattering Mechanism Parameter Values

#### Example

Define an exponential interface trap distribution model named `level`, between Silicon and Oxide. As the `orient` and `carrier` parameters are not set, the definition will match all interfaces for both electrons and holes:

```
define      Silicon.Oxide.level trap_exponential

interface  Silicon.Oxide.level.type acceptor    # Acceptor traps
interface  Silicon.Oxide.level.E0 0.5          # Energy above valence band [eV]
interface  Silicon.Oxide.level.Es 0.4          # Energy range about E0 [eV]
interface  Silicon.Oxide.level.N0 1.0E10        # Trap density [/cm2 /eV]
```

#### Gaussian Interface Trap Distribution

A Gaussian interface trap distribution model allows the association of parameters that describe a Gaussian distribution of traps over an energy range at an interface. In addition to the common parameters (see [Table 15](#)), a `trap_gaussian` model defines the parameters listed here.

*Table 20 Parameters specific to trap\_gaussian model*

Parameter	Description	Type	Default	Unit
E0	Sets the energy of the midpoint of the energy distribution relative to the valence band edge.	float	0.0	eV
Es	Sets the width of the energy range over which the trap density is defined.	float	0.0	eV
N0	Sets the magnitude of the trap density, such that the density is $N(E) = N_0 \exp\left(-\frac{(E - E_0)^2}{2E_s^2}\right)$ .	float	0.0	$\text{cm}^{-2} \text{eV}^{-1}$

#### Example

Define a Gaussian interface trap distribution model named `level`, between Silicon and Oxide. As the `orient` and `carrier` parameters are not set, the definition will match all interfaces for both electrons and holes:

```
define      Silicon.Oxide.level trap_gaussian

interface  Silicon.Oxide.level.type hneutral    # Donor traps
interface  Silicon.Oxide.level.E0 0.9          # Energy above valence band [eV]
interface  Silicon.Oxide.level.Es 0.2          # Energy range about E0 [eV]
interface  Silicon.Oxide.level.N0 1.0E10        # Trap density [/cm2 /eV]
```

## Interface Trap Level Model

An interface trap level model allows the association of parameters that describe the density of traps at a single energy level at an interface. You assign parameters in the input file by using the `interface` command. In addition to the common parameters (see [Table 15](#)), a `trap_level` model defines the parameters listed here.

*Table 21 Parameters specific to trap\_level model*

Parameter	Description	Type	Default	Unit
E0	Sets the energy of the trap relative to the valence band edge.	float	0.0	eV
N0	Sets the magnitude of the trap density, such that the density is $N(E) = N0$ for $E = E0$ .	float	0.0	$\text{cm}^{-2}$

### Example

Define an interface trap level model named `level`, between `Oxide` and `HfO2`. As the `orient` and `carrier` parameters are not set, the definition will match all interfaces for both electrons and holes:

```
define Oxide.HfO2.level trap_level
interface Oxide.HfO2.level.type donor # Donor traps
interface Oxide.HfO2.level.E0 0.2      # Energy above valence band [eV]
interface Oxide.HfO2.level.N0 5.0E10   # Trap density [/cm2]
```

## Tabulated Interface Trap Distribution Model

A tabulated interface trap distribution model allows the association of parameters that describe a user-defined distribution of traps in energy at an interface. In addition to the common parameters (see [Table 15](#)), a `trap_table` model defines the parameter listed here.

*Table 22 Parameter specific to trap\_table model*

Parameter	Description	Type	Default	Unit
table	Specifies a list of energy (eV) and density ( $\text{cm}^{-2}\text{eV}^{-1}$ ) value pairs that define the distribution, such that the density is $N(E) = N_i$ for $E_{i-1} < E \leq E_{i+1}$ .	table	(0.0, 0.0)	eV, $\text{cm}^{-2}\text{eV}^{-1}$

## Chapter 5: Monte Carlo Input File

### Scattering Mechanism Parameter Values

#### Example

Define a tabulated interface trap distribution model named `level`, between Silicon and Oxide. As the `orient` and `carrier` parameters are not set, the definition will match all interfaces for both electrons and holes:

```
define      Silicon.Oxide.level trap_table

interface Silicon.Oxide.level.type hneutral          # Donor traps
interface Silicon.Oxide.level.table E 0.00 piecewise 0.0E11
                                         # 0.0 eV -> 0.1 eV, 0x10^11 /cm2
interface Silicon.Oxide.level.table E 0.10 piecewise 1.0E11
                                         # 0.1 eV -> 0.2 eV, 1x10^11 /cm2
interface Silicon.Oxide.level.table E 0.20 piecewise 5.0E11
                                         # 0.2 eV -> 0.3 eV, 5x10^11 /cm2
interface Silicon.Oxide.level.table E 0.30 piecewise 1.0E11
                                         # 0.3 eV -> 0.4 eV, 1x10^11 /cm2
interface Silicon.Oxide.level.table E 0.40 piecewise 0.0E11
                                         # 0.4 eV ->           , 0x10^11 /cm2
```

#### Uniform Interface Trap Distribution Model

A uniform interface trap distribution model allows the association of parameters that describe a uniform distribution of traps over an energy range at an interface. In addition to the common parameters (see [Table 15](#)), a `trap_uniform` model defines the parameters listed here.

*Table 23 Parameters specific to trap\_uniform model*

Parameter	Description	Type	Default	Unit
<code>E0</code>	Sets the energy of the midpoint of the energy distribution relative to the valence band edge.	float	0.0	eV
<code>Es</code>	Sets the energy range over which the trap density is defined.	float	0.0	eV
<code>N0</code>	Sets the magnitude of the trap density, such that the density is $N(E) = N0$ for $E - \frac{1}{2}Es < E0 < E + \frac{1}{2}Es$ .	float	0.0	$\text{cm}^{-2}\text{eV}^{-1}$

### Example

Define a uniform interface trap distribution model named `level`, between Silicon and Oxide. As the `orient` and `carrier` parameters are not set, the definition will match all interfaces for both electrons and holes:

```
define      Silicon.Oxide.level trap_uniform

interface  Silicon.Oxide.level.type acceptor # Acceptor traps
interface  Silicon.Oxide.level.E0 0.5      # Energy above valence band [eV]
interface  Silicon.Oxide.level.Es 0.4      # Energy range about E0 [eV]
interface  Silicon.Oxide.level.N0 1.0E10 # Trap density [/cm2 /eV]
```

---

### Storing $k \cdot p$ Band Structures

The six-band  $k \cdot p$  valence band structure is precalculated and stored on a polar mesh (see [Six-Band  \$k \cdot p\$  Band Structure Model on page 297](#)). The quantities tabulated by default are  $E(k)$ ,  $k(E)$ , and  $v(k)$ . The default resolution of the band structure is chosen to minimize memory overhead, while ensuring no significant loss of accuracy, and is based on a maximum energy over which  $k(E)$  is tabulated, with the energy and velocity tabulated over consistent ranges. However, you can change the default resolution by using the syntax outlined in [Valley Parameter Values on page 216](#). For example, the following commands in the input file adjust the silicon heavy-hole (HH) band structure to be stored up to an energy of 1 eV and with a resolution in energy of 1 meV:

```
material Silicon.valence.HH.vhh.E-kp    1.0
material Silicon.valence.HH.vhh.bins-kp 1000
```

Again, the resolution of energy and velocity tabulation is consistent with this definition. You can also define a maximum  $k$ -vector for the  $E(k)$  tabulation directly, in units of  $2\pi/a$ :

```
material Silicon.valence.HH.vhh.k-kp 0.5
```

Similarly, the following command in the input file adjusts the scattering rate table associated with the light-hole (LH) band in Ge to tabulate rates over an energy of 1 eV and with a resolution in energy of 1 meV (the resolution is defined internally). The spherically averaged masses are tabulated using the same limits as scattering rates:

```
material Germanium.valence.LH.vlh.rates.E 1.0
```

By default, unstressed materials are tabulated for only one octant of the Brillouin zone (up to the energy or  $k$ -vector limit). With stress applied, four octants are used due to the change in symmetry.

You can define the number of octants used to store a given band structure as follows:

```
material Silicon.valence.octants 4
```

## Chapter 5: Monte Carlo Input File

### Scattering Mechanism Parameter Values

The possible values represent the following:

- 1: Eighth of the zone
- 2: Quarter of the zone
- 4: Half of the zone
- 8: Entire zone

**Note:**

If the material is stressed and fewer than four octants are supplied, then a warning is printed, but the simulation continues.

You can also use a direct calculation for  $E(k)$ . This is slower than tabulating but reduces the memory overhead by approximately 20% based on the default storage parameters. To deactivate tabulation for  $E(k)$ , specify the following in the input file:

```
material Silicon.valence.tabulate_Ek off
```

**Note:**

Using the default resolution (900 bins for 1.0 eV), a single material using all three valleys in the valence band would require ~3 GB memory for the simulation.

## Writing $k \cdot p$ Band Structures to Files

A six-band  $k \cdot p$  valence band structure can be calculated and written to file. Simulations can then read the band structure instead of calculating it, reducing the runtime of the initialization period.

The entire band structure, consisting of the heavy-hole, light-hole, and spin split-off bands, can be written by using the following command:

```
garand-mc -fdd <path_to_mct_file> -f <path_to_input_file> --bands
```

This command results in Garand MC terminating after the band structure is calculated and written to file. Alternatively, you can use the following input file command:

```
material Silicon.valence.<band>.write on
```

This command allows the simulation to proceed with the band structure written as an additional output.

By default, the band structure is written to a single directory within the simulation output directory and named after the experiment.

## Chapter 5: Monte Carlo Input File

### Scattering Mechanism Parameter Values

The directory contains five files per written band that store the band structure, the first derivative, the maximum calculated energy, and the 2D and 3D density-of-states masses. These are named after the material and band as follows:

```
<directory>/<experiment>_kp_bands/
    |--- <material>_<band>_2D_DoS_mass.dat
    |--- <material>_<band>_dEdk.dat
    |--- <material>_<band>_DoS_mass.dat
    |--- <material>_<band>_kE.dat
    |--- <material>_<band>_max_E.dat
```

A nondefault output directory for the calculated band structure can be specified using the following command:

```
material <material>.valence.<band>.write_path <output_directory_path>
```

The output directory path is either a relative path or an absolute path.

## Reading k·p Band Structures From Files

Having calculated and written a band structure to file, you can read the file by using the following input file command:

```
material <material>.valence.<band>.read on
```

This command reads all the band-structure files for all the written bands found within the default output directory. For example, to read a precalculated silicon valence band structure that has been written to the default output directory, use the following command:

```
material Silicon.valence.<band>.read on
```

Any bands not read in are calculated.

If the band structure to be read has been written to a nondefault output directory, then you can specify the path as follows:

```
material <material>.valence.<band>.path <output_directory_path>
```

### Note:

When reading in a precalculated band structure, the mesh and strain conditions specified in the input file must match those used to precalculate the band structure. If there are inconsistencies, then the simulation terminates with an error, and the necessary amendments to the input file will be written to screen. The band structure parameters ( $L$ ,  $M$ , and  $N$ ) do not have to match at this stage.

## Strain

For details about how to apply stress or strain in Garand, see [Material Strain on page 285](#).

---

## Spatially Varying Material Properties

In MC simulations, the impact of spatially varying mole fraction and stress fields is captured in the variation of the band structure with respect to both position and momentum. The real-space propagation is influenced by an additional driving field derived from the variation of the conduction and valence band edges. The impact in momentum space is determined by a band structure calculated from averaged values of the mole fraction and stress field in each region.

## Initial Drift-Diffusion Simulation

To include the impact of spatially varying material parameters in MC simulations, a drift-diffusion simulation must be performed first with additional parameters activated to ensure that the mole fraction and stress fields are read in from the imported TDR file and are used to calculate material parameters.

The variation in mole fraction is accounted for by the following parameter:

```
structure xMoleFraction = on
```

This parameter is activated by default.

The stress field is imported by using the following parameter:

```
strain import = on
```

This parameter is deactivated by default.

For more information, see [Importing an Alloy Fraction on page 90](#) and [Stress and Strain on page 94](#).

Finally, the following parameter specifies how these fields are transferred to Garand MC:

```
simulation pos_dep = on
```

With `pos_dep=on` (default), the material parameters determining the driving field are calculated at each mesh point, based on local values of the mole fraction and the stress field, and are passed to Garand MC using the MCT file.

Deactivating this parameter simplifies the material structure, creating discrete material regions based on the mole fraction, rounded off to the nearest 10% fraction (see [Importing an Alloy Fraction on page 90](#)).

## Driving Field

With `pos_dep=on` for a MC simulation, variation in the conduction and valence band edges is accounted for as an additional driving force during the particle propagation.

The conduction and valence band edges from both Garand and Garand MC can be written to a TDR file for inspection by using the following parameter:

```
output bands = on
```

This parameter is activated by default.

## Band Structure and Scattering

For simulations where a spatially varying mole fraction is accounted for in the additional driving field, the band structure and scattering are defined using a single mole fraction for each region. The syntax to define this is:

```
material <name>.x_fraction 0.53
```

The name can be either a material or region name. In the latter case, all regions will inherit the mole fraction value unless an explicit region definition is defined.

Parameters related to the `interface` command can be defined as usual, also using material or region names.

An additional parameter is available for alloy scattering, where the local mole fraction can be used to define the scattering at any given position, rather than using the fraction defined for the band structure. This can be switched on by using the following input file command:

```
simulation mc_pos_dep_scat = on
```

This parameter is deactivated by default, so all alloy scattering will be based on the average mole fraction in a region.

## Applying Stress

The stress-induced modification to the band structure can be introduced in one of the following ways:

- Use an averaged stress tensor extracted from the stress field from process simulation.
- Modify the input file.

If the flags to import stress and apply position-dependent properties in a MC simulation are set, then the impact of stress is included only through the driving field. To activate the transfer of the averaged stress tensor in each region, change the command as follows:

```
strain import=on transfer_average=on
```

## Chapter 5: Monte Carlo Input File

### Long-Channel Simulations

Stress is then transferred to the MC simulation by using an average stress transfer (.ast) file written to the same directory as the MCT file, and a stress tensor for each region where the stress field is nonzero will be written.

By default, all components of the stress tensor are transferred; however, it is possible to import only the diagonal components of the stress tensor by setting `diagonal_only=on`. The off-diagonal components in this case will be zero.

You can modify the definition in the input file in one of the following ways:

- Instead of the average stress tensor generated from the drift-diffusion simulation
- In addition to the average stress tensor generated from the drift-diffusion simulation

To replace the average tensor, amend the command as follows:

```
strain import=on transfer_average=off
```

This prevents the parsing of the .ast file, and only stress defined in the input file is applied (by default, `transfer_average=off`). With `transfer_average=on`, the value can be overwritten for an individual region or material using the following syntax:

```
strain <name>.device_stress_tensor σxx, σyy, σzz, σyz, σxz, σxy  
transfer_average=off
```

As with mole fraction, a definition using a region name overwrites any definitions based on material names. This is also a means to remove stress from a specific region by setting all components to zero. Nonzero stress tensors for each region are reported to screen and written to the material parameter file in the data directory.

Alternatively, you can change the `strain import` command so that stress definitions in the input file are added to the average transferred from the drift-diffusion simulation. For example:

```
strain import=on additive=on
```

Any stress sources must have a unique name (see [Specifying Multiple Strain Definitions on page 289](#)), and a stress tensor cannot be defined in this case because only one stress tensor per material can be defined.

---

## Long-Channel Simulations

You can simulate MC transport along an infinitely long channel, consistent with the channel defined within a device structure. This is achieved by restricting the simulation domain to a cross section through the channel.

You can use the `autoslice` and `remove_source_drain` parameters to modify the device structure to simulate the channel cross-section only (see [Long-Channel Simulation on page 49](#)).

## Automatically Slicing a Device

The `autoslice` parameter is used to slice a device at its midpoint along the channel. This is the preferred option as it simplifies the procedure for users. For example:

```
simulation autoslice=on
```

This command must be included in the initial drift-diffusion simulation in order for the structure changes to be passed to Garand MC using the MCT file (see [Monte Carlo Transfer Files on page 48](#)).

By default, the source and drain regions are not removed and no field is applied in any direction.

Given the amended structure, periodic boundaries and a driving field must be applied to simulate long-channel mobility. A vector field, in kV/cm, can be applied in a MC simulation by using the following command:

```
simulation applied_field = 1.0 0.0 0.0
```

This command applies a 1 kV/cm field along the x-direction. As transport in this example is directed along the x-direction, only a field applied in this direction is required.

In addition, with `autoslice=on`, self-consistent updating of the field using the Poisson equation is deactivated, as well as the removal or injection of particles at Ohmic contacts. Periodic boundary conditions are also applied along the channel direction.

The channel direction in long-channel simulations is determined in one of the following ways:

- Based on user definition using the syntax:

```
simulation channel_direction=x
```

- Based on the applied field, taking the channel direction as being along that of the largest field

---

## Refining Automatic Slicing

Alternatively, you can use the following command:

```
structure remove_source_drain=on
```

in combination with a physical domain specified by the `mesh` command. For example:

```
mesh import xmin = -0.1 xmax = 1.0
```

## Chapter 5: Monte Carlo Input File

### Streaming Monte Carlo Simulations

This allows a finer degree of control over how the slice is defined. However, this approach requires you to provide more information in the input file in addition to that specified for the `autoslice` method.

Density-gradient boundary conditions at the domain edges must also be enforced, to ensure invariance along the channel, by setting:

```
contact confined_boundary = on
```

Periodic boundaries must be set in the direction of the applied field manually. For example:

```
simulation periodicX = on
```

The default removal or injection of particles at Ohmic contacts must also be suspended as follows:

```
simulation ohm_ctc = off
```

To deactivate self-consistent updating of the field by solving the Poisson equation, use:

```
simulation self_consistent = off
```

---

## Streaming Monte Carlo Simulations

Streaming MC simulations allow you to define a set of initial carrier states and to follow the resulting trajectories within the simulation domain. Any subsequent carriers generated by an initial state, for example, by impact ionization, are simulated together with the initial state in a streaming group. Each particle is simulated independently and not coupled to the Poisson solution.

A limited set of statistics is gathered in this mode. The number of electrons and holes as a function of time, as well as their sum, is written to a file for each simulated streaming group. The time-averaged distribution of electrons and holes within the simulation domain, where the distributions are accumulated from sampling the positions of all simulated carriers in all streaming groups at the end of each time step, is also written to the output TDR file.

---

## Activating Streaming Simulation Mode

To activate the streaming simulation mode, specify the following:

```
simulation MC_mode = stream
```

By default, `MC_mode` is set to `device`, in which case, either an ensemble or a single-particle MC device simulation is executed.

When `MC_mode=stream`, the `ensemble` parameter of the `simulation` command is switched off by default and the `single_particle` parameter is switched on. If you set either

## Chapter 5: Monte Carlo Input File

### Streaming Monte Carlo Simulations

ensemble or single\_particle manually and the set parameter conflicts with these enforced values, then an error is reported and the simulation terminates.

---

## Streaming Grid

In streaming MC simulation mode, the initial carrier positions are defined as nodes within a regularly spaced cuboid grid, using the following input file syntax:

```
structure stream_grid [options]
```

The following options are available:

Parameter	Type	Description	Default	Unit
carrier	string	Sets the initial carrier type. Options are: <ul style="list-style-type: none"><li>• electron</li><li>• hole</li></ul>	electron	–
E	float	Sets the initial carrier energy.	0.001	eV
nx	integer	Sets the number of nodes in the resolving grid along the x-axis.	1 (xmin)	–
ny	integer	Sets the number of nodes in the resolving grid along the y-axis.	1 (ymin)	–
nz	integer	Sets the number of nodes in the resolving grid along the z-axis.	1 (zmin)	–
xmin	float	Sets the position of the lower bound of the streaming grid along the x-axis.	Domain edge	nm
xmax	float	Sets the position of the upper bound of the streaming grid along the x-axis.	Domain edge	nm
ymin	float	Sets the position of the lower bound of the streaming grid along the y-axis.	Domain edge	nm
ymax	float	Sets the position of the upper bound of the streaming grid along the y-axis.	Domain edge	nm
zmin	float	Sets the position of the lower bound of the streaming grid along the z-axis.	Domain edge	nm
zmax	float	Sets the position of the upper bound of the streaming grid along the z-axis.	Domain edge	nm

## **Chapter 5: Monte Carlo Input File**

### Streaming Monte Carlo Simulations

Multiple streaming grids can be defined to initialize an arbitrary number of electron and hole states over an arbitrary region.

---

## **Termination of Streaming Groups**

Initial carrier states and their associated streaming group are not simulated indefinitely. If all carriers within a streaming group leave the simulation domain through contacts, then the streaming group terminates automatically, and a new initial state and associated group are generated. You can also terminate streaming groups by specifying the maximum number of carriers allowed within a group and the maximum propagation time to allocate to a group.

### **Maximum Number of Carriers**

To define the maximum number of carriers allowed within a streaming group, use the following parameter:

```
simulation stream_max_carriers = 2000
```

If a group accumulates more carriers than allowed, then propagation of the group terminates and a new initial carrier is generated.

### **Maximum Propagation Time**

To define the maximum time to follow a streaming group history, use the following parameter, specifying the time in seconds:

```
simulation stream_max_time = 1.e-11
```

If a group history has been followed for longer than the specified time, then propagation of the group terminates and a new initial carrier is generated.

---

## **Streaming Simulation Output**

This section discusses the output of streaming simulations.

### **Breakdown Probability and Time**

By default, the mean diffusion, buildup, and breakdown times, as well as their standard deviations, are written together with the breakdown probability to a TDR file named <experiment>\_breakdown\_probability.tdr.

These values are defined at the nodes of the streaming grid and are interpolated or extrapolated over the MC tensor-product simulation domain grid to define a continuous field.

## Output to Mixed Mesh

The breakdown probability, mean breakdown time, and jitter can optionally be interpolated on to a mixed-element mesh before being written to the output TDR file. To do this, specify the target mixed-element mesh as follows:

```
output mixed_mesh_tdr=<string>
```

where `<string>` is the path to the TDR file of the mixed-element mesh. This allows the distributions from MC simulation to be combined with results from other tools on the same simulation mesh.

## Carrier Distributions

If you set the following command:

```
output MC_results = on
```

then a TDR file for visualization is written as `<experiment>-MC-Output.tdr`. The TDR file maps the potential distribution over the simulation domain together with the time-averaged electron and hole densities accumulated from sampling the positions of all simulated carriers in all streaming groups at the end of each time step.

## History of Streaming Group

A record of the number of electrons and holes as a function of time is written to file for each streaming group. These history files are written to the histories directory and are compressed, using the initial position, initiated carrier type, and iteration to uniquely define the file name as:

```
<x>_<y>_<z>_elec|hole_<iteration>.history.plt.gzip
```

These history files can be postprocessed to extract distributions of diffusion time, buildup time and, therefore, the detection time and jitter.

## Carrier Trajectories in Streaming Group

You can write the trajectories of all carriers associated with all streaming groups to a TDR file by using the following command:

```
output stream_trajectories = on
```

A file named `<experiment>_trajectories.tdr` is created, which contains the trajectories of all carriers in the individual streaming groups as separate geometries. Within each geometry, electron and hole trajectories are grouped as separate materials, while individual electrons and holes are defined as unique regions. Activating and deactivating materials and regions within Sentaurus Visual allows individual carriers to be tracked.

## Chapter 5: Monte Carlo Input File

### References

Fields can be sampled along each trajectory with the following command:

```
output stream_trajectory_fields = <list>
```

where `<list>` is a comma-separated list of available fields to sample, limited to `energy` and `potential`. By default, the propagation time is mapped to the particle trajectories.

**Note:**

Visualization of trajectories might use a lot of disk space if a simulation follows a large number of streaming groups or a large number of carriers per group, or follows trajectories for a long time.

---

## References

- [1] M. Kampl and H. Kosina, “The backward Monte Carlo method for semiconductor device simulation,” *Journal of Computational Electronics*, vol. 17, pp. 1492–1504, 2018.

# 6

## Output Visualization

---

*This chapter discusses visualization of output.*

---

### Initialization Fields

The `output` command in the input file controls visualization of the simulation domain and the Monte Carlo (MC) solution. This command is used to switch on or off output TDR files and to specify which fields from the MC solution are written to file.

The initial simulation domain, consisting of the drift-diffusion solution used to initialize the simulation and initial MC fields, can be output using the following command in the input file:

```
output domain = on
```

This results in the creation of the output TDR file `<experiment>-MC-Input_<device>.tdr` that contains the material within the simulation domain.

Additional fields, including the MC initialization results, can be included in the TDR file by using the following command:

```
output <field> = on
```

where `<field>` can be one of the fields listed in [Table 24](#).

**Note:**

In some cases, activating a field in the input file results in more than one field being included in the TDR file. These are described in the next sections.

*Table 24      Options for `<field>` keyword*

Quantity	<code>&lt;field&gt;</code>	TDR fields
Acceptor doping concentration	<code>acceptors</code>	<code>AcceptorConcentration</code>
Donor doping concentration	<code>donors</code>	<code>DonorConcentration</code>
Net doping concentration	<code>net_doping</code>	<code>DopingConcentration</code>

## Chapter 6: Output Visualization

### Initialization Fields

**Table 24      Options for <field> keyword (Continued)**

Quantity	<field>	TDR fields
Total doping concentration	total_doping	TotalConcentration
Fixed charge concentration	qfix	Fixed_Charge
Mobile carrier concentration	mobile_charge	eDensity eDensity_snapshot hDensity hDensity_snapshot
Potential	potential	ElectrostaticPotential MCElectrostaticPotential_snapshot
Effective quantum potential	quantum_potential	QuantumPotential QuantumPotential_snapshot
Potentials	potentials	ElectrostaticPotential MCElectrostaticPotential_snapshot QuantumPotential QuantumPotential_snapshot
Band edges	bands	Bandgap ElectronAffinity ConductionBandEnergy ValenceBandEnergy
Electron concentration	electrons	eDensity eMCDensity_snapshot
Hole concentration	holes	hDensity hMCDensity_snapshot
Mole fraction	mole_fraction	xMoleFraction
Permittivity	permittivity	DielectricConstant
Field	field	ElectricField ElectricFieldEff
Quasi-Fermi level	fermi	eQuasiFermiEnergy hQuasiFermiEnergy

## Acceptor Doping Concentration

To write the acceptor doping profile of the simulation domain to the initialization TDR file, specify:

```
output acceptors = on
```

The absolute magnitude of the acceptor concentration  $|N_A|$  is written in units of  $\text{cm}^{-3}$ .

---

## Donor Doping Concentration

To write the donor doping profile of the simulation domain to the initialization TDR file, specify:

```
output donors = on
```

The absolute magnitude of the donor concentration  $|N_D|$  is written in units of  $\text{cm}^{-3}$ .

---

## Net Doping Concentration

To write the net doping profile of the simulation domain to the initialization TDR file, specify:

```
output net_doping = on
```

The difference between the magnitudes of the donor and acceptor concentrations  $|N_D| - |N_A|$  is written in units of  $\text{cm}^{-3}$ .

---

## Total Doping Concentration

To write the total doping profile of the simulation domain to the initialization TDR file, specify:

```
output total_doping = on
```

The sum of the magnitudes of the donor and acceptor concentrations  $|N_D| + |N_A|$  is written in units of  $\text{cm}^{-3}$ .

---

## Fixed Charge Concentration

To write the fixed charge profile of the simulation domain, resulting from discrete impurities or traps, to the initialization TDR file, specify:

```
output qfix = on
```

## Chapter 6: Output Visualization

### Initialization Fields

The signed charge density from discrete charges assigned to the simulation mesh is written in units of C/cm<sup>-3</sup>.

---

## Mobile Carrier Concentration

To write the initial mobile-carrier concentration from the drift-diffusion solution and the initialized hole distribution from a MC simulation to the initialization TDR file, specify:

```
output mobile_charge = on
```

The concentration solution is written in units of cm<sup>-3</sup>.

---

## Potential

To write the potential from the initial drift-diffusion solution (`ElectrostaticPotential`), along with the initial potential solution from a self-consistent MC simulation given the initial charge distribution (`MCElectrostaticPotential_snapshot`), to the initialization TDR file, specify:

```
output potential = on
```

The potential is written in units of V.

---

## Effective Quantum Potential

To write the effective quantum potential from the initial drift-diffusion solution (`QuantumPotential`), along with the initial effective quantum potential solution from a self-consistent MC simulation given the initial charge distribution (`QuantumPotential_snapshot`), to the initialization TDR file, specify:

```
output quantum_potential = on
```

The effective quantum potential is written in units of V.

---

## Potentials

To write both the potential and effective potentials from both the initial drift-diffusion solution and the initial solution for MC to the initialization TDR file, specify:

```
output potentials = on
```

### Note:

This command supersedes the commands to write the potential and the effective quantum potential (see [Potential](#) and [Effective Quantum Potential](#)).

## Band Edges

To write the conduction band and valence band edges to the initialization TDR file, specify:

```
output bands = on
```

The band edges are written in units of eV. The electron affinity and the band gap are also written, both in units of eV.

---

## Electron Concentration

To write the initial electron concentration from the drift-diffusion solution (`eDensity`) and the initialized electron distribution before the MC simulation (`eMCDensity_snapshot`) to the initialization TDR file, specify:

```
output electrons = on
```

The electron concentration solution is written in units of cm<sup>-3</sup>.

---

## Hole Concentration

To write the initial hole concentration from the drift-diffusion solution (`hDensity`) and the initialized hole distribution before the MC simulation (`hMCDensity_snapshot`) to the initialization TDR file, specify:

```
output holes = on
```

The hole concentration solution is written in units of cm<sup>-3</sup>.

---

## Mole Fraction

To write the mole fraction profile of the simulation domain to the initialization TDR file, specify:

```
output mole_fraction = on
```

The mole fraction is written to file, ranging from 0 to 1.

---

## Permittivity

To write the permittivity profile of the simulation domain to the initialization TDR file, specify:

```
output permittivity = on
```

## Chapter 6: Output Visualization

### Steady-State Fields

The permittivity is written as a dimensionless quantity to file.

---

## Field

To write the electric field profile of the simulation domain to the initialization TDR file, specify:

```
output field = on
```

The field is written in units of  $\text{Vcm}^{-1}$ .

---

## Quasi-Fermi Level

To write the quasi-Fermi level profile of the simulation domain to the initialization TDR file, specify:

```
output fermi = on
```

The quasi-Fermi level is written in units of eV.

---

## Steady-State Fields

The steady-state period is defined as the simulation time following the user-defined transient (see [Transient Time Steps on page 195](#)). To activate the output of time-averaged fields over this steady-state period to a TDR file for any property, you must specify the following command:

```
output MC_results = on
```

This results in the creation of the output TDR file

`<experiment>-MC-Output_<device>.tdr` that contains the material within the simulation domain.

By default, this TDR file is written only at the end of the simulation, but you can update the file at every intermittent step after the transient (see [Intermittent Time Steps on page 196](#)) by specifying the following command:

```
output update_tdr = on
```

**Note:**

Writing TDR files can have a nonnegligible computational cost, so you might observe a slight increase in runtime when activating this parameter.

Additional fields can be included in the TDR file by using the following command:

```
output <field> = on
```

## Chapter 6: Output Visualization

### Steady-State Fields

The `<field>` keyword is defined for time-averaged potentials and mobile charge, as previously described in [Initialization Fields on page 237](#), and for the time-averaged properties listed in [Table 25](#).

*Table 25 Options for `<field>` keyword*

Quantity	<code>&lt;field&gt;</code>	TDR fields
Carrier energy	energy	eMCEk eMCETot hMCEk hMCETot
Velocity	velocity	eMCVelocity hMCVelocity
Current density	current_density	eMCCurrent hMCCurrent
<i>k</i> -vector	wavevector	eMCKvec hMCKvec
Acceptor doping concentration	acceptors	AcceptorConcentration
Donor doping concentration	donors	DonorConcentration
Net doping concentration	net_doping	DopingConcentration
Total doping concentration	total_doping	TotalConcentration
Mobile carrier properties	carrier_properties	eMCEk eMCETot hMCEk hMCETot eMCCurrent hMCCurrent eMCVelocity hMCVelocity
Potential	potential	ElectrostaticPotential
Effective quantum potential	quantum_potential	QuantumPotential

## Chapter 6: Output Visualization

### Steady-State Fields

Table 25 Options for `<field>` keyword (Continued)

Quantity	<code>&lt;field&gt;</code>	TDR fields
Band edges	<code>bands</code>	<code>Bandgap</code> <code>ElectronAffinity</code> <code>ConductionBandEnergy</code> <code>ValenceBandEnergy</code>
Electron concentration	<code>electrons</code>	<code>eDensity</code> <code>eMCDensity</code>
Hole concentration	<code>holes</code>	<code>hDensity</code> <code>hMCDensity</code>
Field	<code>field</code>	<code>ElectricField</code> <code>ElectricFieldEff</code>
Quasi-Fermi level	<code>fermi</code>	<code>eQuasiFermiEnergy</code> <code>hQuasiFermiEnergy</code>

---

## Carrier Energy

To write the time-averaged carrier kinetic and total energy (mobile carrier species only) to the output TDR file, specify:

```
output energy = on
```

The energy is written in units of eV.

---

## Velocity

To write the time-averaged carrier velocity vector (mobile carrier species only) to the output TDR file, specify:

```
output velocity = on
```

The velocity is written in units of  $10^7 \text{ cms}^{-2}$ .

## Current Density

To write the time-averaged current density vector (mobile carrier species only) to the output TDR file, specify:

```
output current_density = on
```

The current density is written in units of  $\text{A} \mu\text{m}^{-2}$ .

---

## Mobile Carrier Properties

To write the time-averaged energy, velocity, and current density for all simulated mobile carrier species to the output TDR file, specify:

```
output mobile_properties = on
```

---

## Scattering Distribution

Scattering events are always recorded and the total number of events throughout the simulation is tabulated in the intermittent screen output. In addition, scattering events can be recorded on the simulation mesh and written to file for visualization by specifying:

```
output scattering_mesh = on
```

By default, the energy exchanged between carriers and the crystal lattice during inelastic phonon scattering events is accumulated. Phonon absorption is associated with a positive energy exchange; emission is associated with a negative exchange. The net energy exchange is reported in the simulation output TDR file in the field `NetPhononE`, prefixed with `e` for electron scattering and `h` for hole scattering.

The distribution of all scattering events, both inelastic and elastic, can instead be output by additionally specifying:

```
output scattering_count = on
```

In this case, each event is recorded discretely and the total number of events is reported in the simulation output TDR file.

It is further possible to modify these parameters to report the distribution of individual mechanisms, rather than an aggregate, by specifying:

```
output discrete_scattering = on
```

## Output Options

Statistical data written to the output TDR file is gathered over the simulated particle ensemble. By default, data is collected and output for the ensemble as a whole. However, data can be collected and output for carriers within individual bands, separately for carriers moving from source to drain, from drain to source, or by both band and transport direction.

---

### Band Properties

You can output various properties such as the valley occupation, carrier energy, carrier velocity, and the current density vector. You can output these properties independently to the TDR file.

To separate statistics gathering and output over ensembles of particles identified by band, specify the following command:

```
output separate_bands = on
```

All output fields associated with carrier properties are appended with the material and band name, thereby making it possible to better understand the role of intervalley or interband transitions within the simulation.

---

### Ballistic Properties

To separate statistics gathering and output over the ensemble of particles moving from source to drain and the ensemble from drain to source, specify the following command:

```
output ballisticity = on
```

All output fields associated with carrier properties are appended with `pos` to denote that the values are associated with those carriers moving in a positive direction between source and drain, or with `neg` to denote that the values are associated with those carriers moving in the opposite direction.

This information can be used to evaluate the ballisticity of a device from the positive and negative current density. Two simple formulas are required. The first formula evaluates the ratio between the *positive* and net current density at the virtual source:

$$r = \frac{|J^+|}{|J^+| - |J^-|} \quad (50)$$

The second formula evaluates the ballistic ratio (BR):

$$BR = \left( \frac{1-r}{1+r} \right) \quad (51)$$

## Scattering Rates

The calculated scattering rates for the selected material mechanisms within the simulation can optionally be written to file using the following command:

```
output scattering_rates = on
```

File names are created automatically based on the material and mechanism names with the following general form:

```
<experiment>/<scat_dir>/<material>_<band>_<mechanism>.dat
```

---

## Additional Output

This section discusses additional output you can specify in the input file.

---

### Time Evolution

As well as writing a TDR file for visualizing the distribution of steady-state carrier properties within the simulation domain, statistics can be gathered at each time step to write the time evolution of ensemble average carrier properties during the simulation.

To switch on this time evolution output, specify the following command:

```
output time_evolution = on
```

Statistics are gathered over the entire ensemble but can be gathered over individual bands and by direction as with TDR output using the following commands:

```
output separate_bands = on  
output ballisticity = on
```

Output files are written to the MC data directory:

```
<output_directory>/<experiment_name>/data/
```

---

## Energy and Wavevector Distributions

The steady-state distribution of the carrier energy and wavevector can be output by specifying the following commands:

```
output E_distribution = on  
output k_distribution = on
```

When output of the energy distribution is activated, two files are written for each simulated carrier type, which contain, separately, the kinetic energy and the total energy distributions

## Chapter 6: Output Visualization

### Additional Output

along the channel direction. These files are named `eEkDist.tdr` and `eEtDist.tdr` for electrons and `hEkDist.tdr` and `hEtDist.tdr` for holes. In addition to the energy distributions, the average kinetic energy along the channel is defined as a 1D grid within the kinetic energy distribution file, while the average total energy and the average band edge are defined within the total energy distribution file.

The maximum energy, in eV, and the energy resolution of electron and hole distributions, defined by the number of bins between 0 and the maximum energy, can be specified with the following commands:

```
output max_E_el = <float>
output max_E_ho = <float>

output N_dist_el = <integer>
output N_dist_ho = <integer>
```

For the total energy distribution, the maximum energy defined here is applied to the maximum potential energy profile along the channel to set an upper bound to the distribution, and the lower bound is set by the minimum potential energy. Therefore, the resolution in energy depends on this range, which is sensitive to applied and built-in biases.

The output files are written to the `MC data` directory:

```
<output_directory>/<experiment_name>/data/
```

---

## Averaged and Integral Cutlines

Garand MC outputs averaged or integral quantities along the channel similar to Garand as described in [Extracting Integrated and Averaged Cutline Data on page 173](#). Available options are described here. Each quantity is written to the `data` directory:

```
<output_directory>/<experiment_name>/data/
```

## Integral Charge Density

You can write the carrier density, in cross sections across the device, integrated over the cross-sectional area to an output file in the `data` directory. The output units are  $\text{cm}^{-1}$ .

To switch on this output, specify:

```
output integral_charge = on
```

For NFET simulations, the output files are `line_density_dd_el.dat` for the initial guess and `line_density_el.dat` for the MC output. For PFET simulations, the equivalent output files are `line_density_dd_ho.dat` and `line_density_ho.dat`.

## Chapter 6: Output Visualization

### Additional Output

## Weighted Average Velocity

You can write the average velocity in cross sections across the device, weighted by the carrier density, to an output file in the `data` directory. The output units are  $\text{ms}^{-1}$ .

To switch on this output, specify:

```
output weighted_velocity = on
```

For NFET simulations, the output file is `weighted_velocity_el.dat`. For PFET simulations, the output file is `weighted_velocity_ho.dat`.

## Limiting the Integration Range

You can limit the integration or averaging range to cover only a specific part of the device structure.

You specify the limits of the integration range with the following parameters, where `<value>` is the integration range limit (in nm) in the considered direction:

```
output integration_xmin = <float>
output integration_xmax = <float>
output integration_ymin = <float>
output integration_ymax = <float>
output integration_zmin = <float>
output integration_zmax = <float>
```

---

## Visualizing Band Structures

To plot  $E(k)$  dispersion, use the following command:

```
output band_dispersions = on
```

Then, the line along which the dispersion is plotted can be defined by specifying start and end points in  $k$ -space as follows:

```
output kvecline lineName=<string> start=<x> <y> <z> end=<x> <y> <z>
```

Each line has a unique name, and the start and end points are given in units of  $(2\pi/a, 2\pi/b,$  and  $2\pi/c)$  for semiconductors with a zinc-blende lattice and  $(2\pi/\sqrt{3}a, 4\pi/3b,$  and  $2\pi/c)$  for semiconductors with a wurtzite lattice, where  $a, b,$  and  $c$  are the lattice constants. Additional parameters can be supplied to filter based on band container, valley, material, and region. For example:

```
output kvecline lineName=<string> start=<x> <y> <z> end=<x> <y> <z>
          band=conduction | valence
output kvecline lineName=<string> start=<x> <y> <z> end=<x> <y> <z>
          valley=<list_of_valley_names>
output kvecline lineName=<string> start=<x> <y> <z> end=<x> <y> <z>
          material=<list_of_material_names>
```

## Chapter 6: Output Visualization

### Additional Output

```
output kvecline lineName=<string> start=<x> <y> <z> end=<x> <y> <z>
region=<list_of_region_names>
```

Combinations of these parameters can be defined to tailor the output and, by default, all materials or regions and valleys will be written (one file per line, valley, material, or region).

Dispersions are written for the conduction band if `sim_elecs=on` and for the valence band if `sim_holes=on`.

If `band_dispersions=on` but you do not define any lines, then a set of default lines is written (see [Table 26](#)).

*Table 26 Default lines in k-space along which energy dispersions are written*

Name	Start	End	Notes
k1	[000]	$\text{k\_vec\_kp\_disp} \times \hat{x}$	Intended to visualize the $\Gamma$ -valleys; written for both <code>sim_elecs=on</code> and <code>sim_holes=on</code> .
k2	[000]	$\text{k\_vec\_kp\_disp} \times \hat{y}$	Intended to visualize the $\Gamma$ -valleys; written for both <code>sim_elecs=on</code> and <code>sim_holes=on</code> .
k3	[000]	$\text{k\_vec\_kp\_disp} \times \hat{z}$	Intended to visualize the $\Gamma$ -valleys; written for both <code>sim_elecs=on</code> and <code>sim_holes=on</code> .
k4	[000]	[100]	Intended to visualize the $\Delta$ -valleys; written only for <code>sim_elecs=on</code> .
k5	[000]	[010]	Intended to visualize the $\Delta$ -valleys; written only for <code>sim_elecs=on</code> .
k6	[000]	[001]	Intended to visualize the $\Delta$ -valleys; written only for <code>sim_elecs=on</code> .
k7	[000]	[111]	Intended to visualize the $L$ -valleys; written only for <code>sim_elecs=on</code> .
k8	[000]	[111]	Intended to visualize the $L$ -valleys; written only for <code>sim_elecs=on</code> .
k9	[000]	[111]	Intended to visualize the $L$ -valleys; written only for <code>sim_elecs=on</code> .
k10	[000]	[111]	Intended to visualize the $L$ -valleys; written only for <code>sim_elecs=on</code> .

## Chapter 6: Output Visualization

### Additional Output

The `k_vec_kp_disp` parameter is a scaling factor in units of  $2\pi/a$ , which is 0.5 by default. It can be specified using:

```
output k_vec_kp_disp = 0.5
```

Here,  $\hat{x}$ ,  $\hat{y}$ , and  $\hat{z}$  are the normalized vectors denoting the device orientation. The resulting dispersions are written to files in the `viz` directory, with the following naming convention:

```
<experiment>_<region>_<valley>_<line>_energy.plt
```

where `<experiment>`, `<region>`, `<valley>`, and `<line>` are the names of the experiment, region, valley, and line. As each region can contain only one material, if the material filter is applied, then the files will still be named after the region.

In addition, this assumes that valleys in the conduction band and the valence band do not share the same name.

Table 27 Fields written to output PLT file to visualize band structure  $E(k)$  dispersions

Label	Description	Unit
energy	Energy, measured relative to the top of the valence band	eV
DeltaK	The x-coordinate between 0 and 1	—
kmag	Magnitude of the $k$ -vector	Dependent on lattice type
kx	The x-component of the $k$ -vector	Dependent on lattice type
ky	The y-component of the $k$ -vector	Dependent on lattice type
kz	The z-component of the $k$ -vector	Dependent on lattice type

# 7

## Monte Carlo Simulation Models

---

*This chapter describes the models relevant to Monte Carlo simulations.*

---

### Assigning Charges

The cloud-in-cell (CIC) scheme [1] is used to assign all Monte Carlo (MC) simulation particle charges to the simulation mesh. The CIC scheme is applied consistently throughout the mesh. Although proposed hybrid charge assignment schemes such as nearest-element-center (NEC) [2] can be adopted, they are not implemented.

---

### Interpolating Force

Calculation of the force at a particle position within the mesh uses a trilinear interpolation of the displacement fields calculated at the eight nodes that define the cell within which the particle is found. Such a scheme is consistent with the charge assignment and minimizes self-forces [1].

Displacement fields at each mesh point are calculated using a three-point centered difference approximation of the potential derivative following [3]. The x-, y-, and z-components of the displacement field at mesh point  $i, j, k$  with position  $(x, y, z)_{i,j,k}$  are given, respectively, by:

$$(D_x)_{i,j,k} = \frac{1}{2} \left( \frac{\epsilon_{i-1,j,k}(\Psi_{i-1,j,k} - \Psi_{i,j,k}) + \epsilon_{i,j,k}(\Psi_{i,j,k} - \Psi_{i+1,j,k})}{x_{i,j,k} - x_{i-1,j,k}} \right) \quad (52)$$

$$(D_y)_{i,j,k} = \frac{1}{2} \left( \frac{\epsilon_{i,j-1,k}(\Psi_{i,j-1,k} - \Psi_{i,j,k}) + \epsilon_{i,j,k}(\Psi_{i,j,k} - \Psi_{i,j+1,k})}{y_{i,j,k} - y_{i,j-1,k}} \right) \quad (53)$$

$$(D_z)_{i,j,k} = \frac{1}{2} \left( \frac{\epsilon_{i,j,k-1}(\Psi_{i,j,k-1} - \Psi_{i,j,k}) + \epsilon_{i,j,k}(\Psi_{i,j,k} - \Psi_{i,j,k+1})}{z_{i,j,k} - z_{i,j,k-1}} \right) \quad (54)$$

Then, the electric field is calculated by scaling the interpolated displacement field by the local dielectric  $\epsilon$  defined for the cell within which the particle is found.

In [Equation 52](#), [Equation 53](#), and [Equation 54](#),  $\psi$  is either the classical potential or the effective quantum potential (see [Quantum Corrections on page 257](#)), depending on whether the simulation is performed with or without quantum corrections (see [Density-Gradient Quantum Corrections on page 122](#)).

---

## Particle Initialization

Particle initialization defines the initial state of the simulation particles. The state of each particle is defined completely by its position and wavevector. Particles are initialized at the start of a MC simulation and also upon injection into the simulation domain using Ohmic contacts. An equilibrium energy distribution is assumed for initializing all particles at the start of the simulation, but contact injection can use a velocity-weighted distribution to describe the distribution of carriers entering the simulation domain.

---

## Position

MC simulation particles representing electron and hole distributions are initialized within the simulation domain given initial, continuous, carrier densities. The initial distribution typically results from an earlier drift-diffusion solution over the simulation domain. The exception is when a MC simulation is restarted using checkpoint data, in which case, the simulation particle distributions are given explicitly.

---

## Energy

Particle energies are initialized randomly and with a probability consistent with a required energy distribution using the *direct technique* [4]. If  $f_0(E)$  is the required statistical distribution function and  $g(E)$  is the density-of-states (DOS) corresponding to the band in which the particle should be initialized, the required energy distribution function is given by:

$$f(E) = g(E)f_0(E) \quad (55)$$

Using the direct technique, an energy  $E_r$  can be related to a uniform random deviate  $r$ , where  $r \in [0, 1]$ , as:

$$r = \frac{\int_0^{E_r} f(E)dE}{\int_0^{\infty} f(E)dE} \quad (56)$$

from which  $E_r$  will be selected with a probability in accordance with the normalized energy distribution function.

The required energy distribution  $f_0(E)$  is chosen dependent on whether particles are initialized in equilibrium or injected into the simulation domain. Each case is discussed next.

## Equilibrium Energy Distribution

This section discusses equilibrium energy distribution.

### Effective Mass Approximation

For a band modeled by multiple analytic degenerate nonparabolic valleys (see [Analytic Valley Model on page 293](#)), the DOS  $g(E)$  is given by:

$$g(E) = \frac{\sqrt{2}}{\pi^2 \hbar^3} \sum_i \begin{cases} Z_i m_i^* \sqrt{m_i(E - E_i)(1 + \alpha_i(E - E_i))} (1 + 2\alpha_i(E - E_i)) & E \geq E_i \\ 0 & \text{Otherwise} \end{cases} \quad (57)$$

where:

- $E_i$  is the energy minimum.
- $m_i$  is the DOS effective mass.
- $\alpha_i$  is the nonparabolicity factor of the  $i^{\text{th}}$  valley.

The equilibrium statistical distribution function  $f_0$  is the Fermi–Dirac distribution:

$$f_0 = \left( \exp\left(\frac{E - E_F}{k_B T}\right) + 1 \right)^{-1} \quad (58)$$

which can be approximated by the Boltzmann factor  $f_0 = \exp\left(-\frac{E - E_F}{k_B T}\right)$  for  $E \gg E_F$ .

### Fermi–Dirac Distribution

When using Fermi–Dirac statistics, integration over the energy distribution function  $f(E)$  within [Equation 56](#) is defined as:

$$\int_0^{E_r} f(E) dE = \frac{\sqrt{2}(k_B T)^{3/2}}{\pi^2 \hbar^3} \sum_i Z_i m_i^{3/2} \int_0^{\chi_r} \sqrt{\chi} \left( 1 + \frac{5}{2} \alpha_i k_B T \chi \right) (\exp(\chi + \chi_i - \eta) + 1)^{-1} d\chi \quad (59)$$

where  $\chi_r = \frac{E_r}{k_B T} \chi = \frac{E}{k_B T} \chi_i = \frac{E_i}{k_B T} \eta = \frac{E_F}{k_B T}$ .

Here,  $E_r$  is the limit of integration over energy  $E$ ,  $E_i$  is the energy minima of the  $i^{\text{th}}$  valley, and  $E_F$  is the Fermi energy.

Integration over the entire distribution,  $\chi_r = \infty$ , yields the particle density:

$$n = 2 \left( \frac{k_B T}{2\pi \hbar^2} \right)^{\frac{3}{2}} \sum_i Z_i m_i^{3/2} \left( F_{1/2}(\eta - \chi_i) + \frac{15}{4} \alpha_i k_B T F_{3/2}(\eta - \chi_i) \right) \quad (60)$$

## Chapter 7: Monte Carlo Simulation Models

### Particle Initialization

where  $F_j$  is the complete Fermi–Dirac integral of order  $j$ .

Given a uniform random deviate  $r$  and using the direct technique, [Equation 56](#), the random initialization energy  $E_r = k_B T \chi_r$  is given by:

$$\sum_i Z_i m_i^{3/2} \int_0^{\chi_r} \sqrt{\chi} \left(1 + \frac{5}{2} \alpha_i k_B T \chi\right) (\exp(\chi + \chi_i - \eta) + 1)^{-1} d\chi - r \frac{n \sqrt{\pi}}{2} = 0 \quad (61)$$

where  $\chi_r$  is solved numerically by root finding.

### Boltzmann Distribution

When using Boltzmann statistics, integration over the energy distribution function  $f(E)$  within [Equation 56](#) is defined as:

$$\int_0^{E_r} f(E) dE = \frac{\sqrt{2}(k_B T)^{3/2}}{\pi^2 \hbar^3} \exp(\eta) \sum_i Z_i m_i^{3/2} \exp(-\chi_i) \left[ \frac{\sqrt{\pi}}{2} A_i \operatorname{erf}(\chi_r) - \exp(-\chi_r) \left( A_i \sqrt{\chi_r} + \frac{5}{2} \chi_r^{3/2} \right) \right] \quad (62)$$

$$\text{where } A_i = 1 + \frac{15}{4} \alpha_i k_B T \chi_r = \frac{E_r}{k_B T} \chi = \frac{E}{k_B T} \chi_i = \frac{E_i}{k_B T} \eta = \frac{E_F}{k_B T}.$$

Here,  $E_r$  is the limit of energy integration,  $E$  is the energy,  $E_i$  is the minimum energy of the  $i^{\text{th}}$  valley, and  $E_F$  is the Fermi energy.

Integration over the entire distribution,  $\chi_r = \infty$ , yields:

$$n = 2 \left( \frac{k_B T}{2\pi\hbar^2} \right)^{3/2} \sum_i Z_i m_i^{3/2} \exp(\chi_C - \chi_i) \left( 1 + \frac{15}{4} \alpha_i k_B T \right) \exp(\eta - \chi_C) \quad (63)$$

where  $E_C = \chi_C k_B T$  is the energy of the conduction band edge.

Given a uniform random deviate  $r$  and using the direct technique, [Equation 56](#), the random initialization energy  $E_r = k_B T \chi_r$  is given by:

$$\exp(\eta) \sum_i Z_i m_i^{3/2} \exp(-\chi_i) \left[ \frac{\sqrt{\pi}}{2} A_i \operatorname{erf}(\chi_r) - \exp(-\chi_r) \left( A_i \sqrt{\chi_r} + \frac{5}{2} \chi_r^{3/2} \right) \right] - r \frac{n \sqrt{\pi}}{2} = 0 \quad (64)$$

where  $E_r = k_B T \chi_r$  is solved numerically by root finding.

### Six-Band $k \cdot p$ Band Structure

The approach to initializing carriers in an analytic valley is replicated for carriers in a six-band  $k \cdot p$  band structure in which a spherically averaged DOS effective mass is used.

## Equilibrium Velocity

This section discusses equilibrium velocity.

### Effective Mass Approximation

The magnitude of the Herring–Vogt transformed particle wavevector is determined given a randomly generated particle energy with required distribution (see [Equilibrium Energy Distribution on page 254](#)). The wavevector is oriented randomly by selecting two polar angles:

$$\theta = \arccos(1 - 2r) \quad (65)$$

$$\phi = 2\pi r \quad (66)$$

before the inverse Herring–Vogt transform is used to obtain the initialized wavevector.

### Six-Band $\mathbf{k} \cdot \mathbf{p}$ Band Structure

Given a randomly generated particle energy with required distribution, the particle wavevector is selected randomly such that it is weighted by the local DOS in the six-band  $\mathbf{k} \cdot \mathbf{p}$  band structure for states with the required energy (see [Equilibrium Energy Distribution on page 254](#)). This is achieved by applying a rejection procedure on carrier wavevectors initialized isotropically following [Equation 65](#) and [Equation 66](#).

## Contact Injection

Ohmic contact boundaries allow particle flux in and out of the simulation domain (see [Ohmic Contacts on page 262](#)). To maintain the charge density within the simulation domain, the net *out flux* of particles must be balanced by a net *in flux* through a particle injection scheme [5].

Particles are injected assuming an equilibrium distribution. This assumes the out flux that the injection balances is also an equilibrium distribution. Depending on the band structure and the orientation of the injection surface normal  $\mathbf{n}$  with respect to it, particles cross the surface with an average velocity  $\langle v \rangle_n$ .

The number of particles  $N$ , with charge  $q$ , injected over a contact surface at the end of time step  $\Delta t$  is then given by:

$$N = \frac{1}{q} \sum_i \rho_i A_i \langle v \rangle_n \Delta t \quad (67)$$

The summation over  $i$  is over the Ohmic contact boundaries with surface area  $A_i$  and local carrier charge density  $\rho_i$ .

For decoupled contacts, where injection is not defined to be coincident with the contact, the local variation in potential modifies the equilibrium distribution. This is reflected in the

dependence on local density and velocity that define a position-dependent flux. The average injection velocity  $\langle v \rangle_n$  is calculated for arbitrary band structures and orientations.

Carriers injected into a contact contribute to the net charge flux associated with the contact over the previous time step.

---

## Quantum Corrections

In Garand MC, quantum corrections are implemented based on the density gradient approach [6]. Previously, it was difficult to incorporate this form of quantum correction in particle-based simulations due to its sensitivity to noise [7], but this has been resolved [8].

---

### Static Quantum Correction

A static quantum-correction field,  $\psi_{qc}$ , where mapping to the 3D simulation domain is implied, is defined from a self-consistent quantum-corrected drift-diffusion simulation as:

$$\psi_{qc} = \psi_{cl} - \psi_{dg} \quad (68)$$

where the difference is taken between the classical potential  $\psi_{cl}$  from the solution of the nonlinear Poisson equation and the self-consistent density-gradient effective quantum potential  $\psi_{dg}$ . This quantum correction field is determined at the start of the MC simulation and remains fixed throughout.

---

### Quantum-Corrected Potential

The static quantum correction defined by Equation 68 is used to define the quantum-corrected potential field within a MC simulation, at some simulation time  $t$ , as:

$$\psi_{dg}|_t = \psi_{cl}|_t + \psi_{qc} \quad (69)$$

and the subsequent field used to drive particles as:

$$F|_t = -\nabla\psi_{dg}|_t \quad (70)$$

### Frozen-Field Simulation

In a frozen-field simulation, the classical potential  $\psi_{cl}|_t$  in Equation 69 is constant throughout the simulation. Consequently, the density gradient-corrected potential  $\psi_{dg}|_t$  is also constant and equal to the self-consistent density-gradient effective quantum potential from the drift-diffusion simulation.

## Self-Consistent Simulation

In a self-consistent simulation, the classical potential  $\psi_{\text{cl}}|_t$  in [Equation 69](#) is a function of the simulation time step. Variation in  $\psi_{\text{cl}}|_t$  with time is subsequently reflected in the density gradient–corrected potential  $\psi_{\text{dg}}|_t$  by using the static quantum correction.

Both frozen-field and self-consistent corrections capture the relevant quantum effects, in terms of the shift in the peak of the carrier distribution away from the semiconductor–insulator interface and the resulting shift in threshold voltage, while maintaining computation stability and the necessary self-consistency between transport and field.

## Particle Propagation

This section discusses aspects of particle propagation.

### Free Flight

Particles are propagated using the velocity Verlet algorithm, which takes a particle at time  $t$  with position  $\mathbf{r}_t$  and wavevector  $\mathbf{k}_t$ , and defines a new position  $\mathbf{r}_{t+\Delta t}$  and wavevector  $\mathbf{k}_{t+\Delta t}$  at a time  $t + \Delta t$ . Updating the particle wavevector utilizes the field at particle positions both at the start and the end of a time step, while updating the position utilizes the velocity at the midpoint of the time step. This is expressed by the following relationships:

$$\begin{aligned}\mathbf{k}_{t+\Delta t/2} &= \mathbf{k}_t + \frac{1}{\hbar} q \nabla_{\mathbf{r}} V(\mathbf{r}_t) \Delta t / 2 \\ \mathbf{r}_{t+\Delta t} &= \mathbf{r}_t + \frac{1}{\hbar} \nabla_{\mathbf{k}} \epsilon(\mathbf{k}_{t+\Delta t/2}) \Delta t \\ \mathbf{k}_{t+\Delta t} &= \mathbf{k}_{t+\Delta t/2} + \frac{1}{\hbar} q \nabla_{\mathbf{r}} V(\mathbf{r}_{t+\Delta t}) \Delta t / 2\end{aligned}\tag{71}$$

The velocity Verlet algorithm is second-order accurate and time centered. It synchronizes particle coordinates at the end of the time step and uses only one force evaluation per solution of the Poisson equation.

### Interrupted Scattering

Scattering events break the propagation cycle by instantaneously altering the wavevector  $\mathbf{k}$  between  $t$  and  $t + \Delta t$ . Since information regarding the new field cannot be obtained until the result of the scattering event is obtained, propagation to a scattering event during a time step can utilize only the initial field. Some error and loss of time centering is introduced by this deviation from the propagation cycle, although this is neglected as it is not expected that propagating back will recover the state before scattering.

## Simulation Domain Boundaries

Given the simulation domain, several boundary types between mesh cells are defined automatically, depending on material types and boundary conditions. The dynamics of particles encountering cell boundaries are determined by the boundary type and handled according to the following models.

---

### Hitting a Boundary

Particle propagation over a time interval  $\Delta t$  results in an uninterrupted ballistic trajectory with position  $\Delta r$  and momentum  $\Delta k$  increments. If  $\Delta r$  crosses a cell boundary, then the particle is considered to have hit the cell boundary at some time  $t' < \Delta t$ . The time  $t'$  at which the particle arrives at the boundary is found by an iterative search since the propagation algorithm is nonlinear in time (see [Particle Propagation on page 258](#)). Propagation resumes for the remaining time  $\Delta t - t'$  after some action is performed, depending on the boundary type.

Boundary types and their models are defined here.

---

### Heterojunction Boundaries

Mesh cell interfaces between two different semiconductor materials or regions define a heterojunction boundary. Particle transmission across the boundary and into a new semiconductor material is considered purely classically by ensuring both conservation of energy, taking into account energy offsets between materials or regions, and conservation of momentum parallel to the heterojunction. An incident particle is reflected from the heterojunction if a state satisfying these conditions within the new semiconductor material cannot be found.

For all band structures, an energy-conserving and a momentum-conserving state in the new semiconductor material is sought. Suitable transmission states are defined as those with the required final energy and with a velocity directed into the new material.

For six-band  $k \cdot p$  band structures, a final state is sought that lies along an impulse vector that is normal to the interface and applied to the incident particle wavevector within the band structure of the new material.

For analytic band structures based on the effective mass approximation (EMA), this momentum conservation is relaxed somewhat, and a final state is sought that lies along an impulse vector normal to the interface but is applied to the incident wavevector, relative to the occupied valley in the initial material, in all available final valleys. Multiple solutions can be found in this way and the final state is selected randomly, weighted by the final DOS.

## Chapter 7: Monte Carlo Simulation Models

### Simulation Domain Boundaries

In both cases, the magnitude of the impulse is sought and serves only to enforce parallel momentum conservation, becoming defined only when finding a valid state.

## Effective Mass Approximation

Given a band model composed of multiple analytic valleys, energy- and momentum-conserving final states are sought in all valleys by solving for an impulse normal to the heterojunction:

$$\mathbf{k}' = \mathbf{k} + Fdt\hat{\mathbf{n}} = \mathbf{k} + I\hat{\mathbf{n}} \quad (72)$$

with the constraint of energy conservation such that  $\varepsilon'(\mathbf{k}') = \varepsilon(\mathbf{k}) + \Delta\varepsilon'$ .

Here,  $\Delta\varepsilon'$  is the energy difference between the initial valley and the final valley. In all cases, the momentum  $\mathbf{k}$  and the unit normal vector  $\hat{\mathbf{n}}$  are those defined within the Herring–Vogt transformed space associated with the final valley.

The magnitude of the impulse  $I$  is given by the solution of the following quadratic:

$$AI^2 + BI + C = 0 \quad (73)$$

where  $A$ ,  $B$ , and  $C$  are defined as:

$$\begin{aligned} A &= 1 \\ B &= 2k_{\perp} \cdot \hat{\mathbf{n}} \\ C &= k_{\perp}^2 - k'^2 \end{aligned} \quad (74)$$

In [Equation 72](#) to [Equation 74](#), unprimed symbols refer to values within the initial valley (in the initial material), while primed symbols refer to values within the proposed final valley in the final material. All vectors are defined with reference to the crystallographic reciprocal basis vectors, and the final wavevector is defined with respect to the final valley minima.

If no solutions to the quadratic equation ([Equation 73](#)) are found, then energy and momentum conservation is not satisfied and the particle is reflected. If two numeric solutions are found, then the solution that preserves the velocity of the carrier across the heterojunction boundary is chosen.

## Six-Band $k\cdot p$ Band Structure

Within the six-band  $k\cdot p$  band structure, a numeric search in  $k$ -space along the impulse vector is performed analogously to the analytic solutions described in [Effective Mass Approximation on page 260](#).

## Tabulated Band Structure

When you use an imported tabulated band structure, a numeric search in  $k$ -space along the impulse vector is performed analogously to the analytic solutions described in [Effective Mass Approximation on page 260](#).

## Reflective Boundaries

Mesh cell interfaces between semiconductor and insulator materials are treated as a limiting case of the heterojunction boundary discussed in [Heterojunction Boundaries on page 259](#). The conduction band and valence band differences are modeled as abrupt infinite potential barriers, resulting in an impulse normal to the cell boundary. The interaction is treated as instantaneous and elastic, with the impulse applied to the crystal momentum of the carrier, resulting in a final state with velocity directed away from the interface.

For both analytic and six-band  $k \cdot p$  band structures, the final energy- and momentum-conserving states sought are defined as those with the required final energy that lie along the impulse vector normal to the interface and with velocity directed away from the boundary.

## Effective Mass Approximation

Within an analytic band model, the valley in which a particle resides is assumed fixed during reflection. An energy- and momentum-conserving final state is sought in the particle valley by solving for an impulse normal to the heterojunction as in the analytic band treatment of heterojunctions (see [Effective Mass Approximation on page 260](#)):

$$\mathbf{k}' = \mathbf{k} + Fdt\hat{\mathbf{n}} = \mathbf{k} + I\hat{\mathbf{n}} \quad (75)$$

with the constraint of an elastic interaction such that  $\varepsilon(\mathbf{k}') = \varepsilon(\mathbf{k})$ .

The magnitude of the impulse  $I$  is then defined for an analytic valley as:

$$I = \frac{2(k_x \hat{n}_x^* m_y^* m_z^* + k_y \hat{n}_y^* m_x^* m_z^* + k_z \hat{n}_z^* m_x^* m_y^*)}{\hat{n}_x^* m_y^* m_z^* + \hat{n}_y^* m_x^* m_z^* + \hat{n}_z^* m_x^* m_y^*} \quad (76)$$

where  $\hat{\mathbf{n}} = (\hat{n}_x, \hat{n}_y, \hat{n}_z)$  is the interface unit normal in the longitudinal and transverse coordinate systems of the valley, and  $\mathbf{k} = (k_x, k_y, k_z)$  is the incident wavevector. Here,  $x$  is assumed to be the longitudinal axis, and  $y$  and  $z$  are the two transverse axes.

## Six-Band $k \cdot p$ Band Structure

Unlike the analytic valley model, the magnitude of the impulse cannot be obtained directly within the six-band  $k \cdot p$  band structure. A search routine is used to find the first energy-conserving state along the trajectory in momentum space defined by the impulse that has velocity directed away from the interface. This then defines the final state.

---

## External Boundaries

For efficiency, it can be preferable to simulate only half the device structure, and then double the resulting current so that it is representative of the entire-width device simulation. This

## Chapter 7: Monte Carlo Simulation Models

### Simulation Domain Boundaries

allows a smaller mesh and a reduced number of particles to be used, which can reduce the runtime to half that of an equivalent entire device simulation.

To allow this, the reflective boundary conditions at external boundaries in Garand MC are modified versions of the approach used for internal reflective boundaries previously described. These boundary conditions maintain a zero-flux condition across this boundary by taking advantage of the symmetry of the band structure, finding a reflected state that mirrors the incident state.

This approach works well over a wide range of device orientations and materials. However, some care should be taken in certain cases where the symmetry of the band structure might inhibit this approach. For example, for a <111> channel orientation or where stress is not applied parallel to the channel direction, there might be a slight difference in the current when compared to a simulation with the entire device structure. This difference is typically small, no more than 1–2%, and might be acceptable in exchange for a reduction in runtime.

Errors in the simulation setup can also influence the accuracy of a reduced device structure simulation, so always follow best practices (see [Selection of Simulation Parameters and Troubleshooting on page 200](#)).

**Note:**

In Version R-2020.09 of Garand MC, internal boundary conditions were applied at external boundaries. If you need to reproduce this behavior, use the following command:

```
SIMULATION reflect_ext = off
```

However, this is not recommended unless for backward compatibility. In most cases, the default simulation setup should match previous releases.

---

## Ohmic Contacts

Ohmic contact boundaries are defined automatically at mesh cell interfaces between semiconductor materials and regions of fixed potential. If a decoupled region is defined, either automatically associated with a contact (see [Decoupled Contacts on page 205](#)) or manually to overlap a contact (see [Decoupled Regions on page 207](#)), then Ohmic contact boundaries are defined over the surface of the decoupled region. Carriers passing through an Ohmic contact boundary are removed from the simulation domain, and their contribution to the net charge flux through the associated device contact at that time step is accumulated.

The removal of particles through Ohmic contact boundaries is balanced by particle injection over the same boundaries (see [Contact Injection on page 256](#)).

---

## Surface Roughness (Scattering Rate)

Material interfaces can define a nonzero root mean square (RMS) amplitude and correlation length depending on the default materials that form the interface. Independent surfaces within the simulation domain that define a rough surface result in the addition of surface scattering mechanisms to the semiconductor materials that form the interface.

Multiple interfaces result in multiple surface roughness scattering mechanisms, each associated with a single interface. Scattering is valid only if the projection of the position of the particle, normal to the surface, falls within the bounds of the surface.

---

## References

- [1] R. W. Hockney and J. W. Eastwood, *Computer Simulation Using Particles*, New York: Taylor & Francis, 1988.
- [2] S. E. Laux, "On Particle-Mesh Coupling in Monte Carlo Semiconductor Device Simulation," *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems*, vol. 15, no. 10, pp. 1266–1277, 1996.
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- [4] C. Jacoboni and P. Lugli, *The Monte Carlo Method for Semiconductor Device Simulation*, Computational Microelectronics, Wien: Springer, 1989.
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- [7] B. Winstead, H. Tsuchiya, and U. Ravaioli, "Comparison of Quantum Corrections for Monte Carlo Simulation," *Journal of Computational Electronics*, vol. 1, no. 1–2, pp. 201–207, 2002.
- [8] C. Riddet *et al.*, "Simulation of "Ab Initio" Quantum Confinement Scattering in UTB MOSFETs Using Three-Dimensional Ensemble Monte Carlo," *IEEE Transactions on Electron Devices*, vol. 58, no. 3, pp. 600–608, 2011.

## **Part III: Material Models**

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This part of the *Garand User Guide* contains the following chapters:

- [Chapter 8, Semiconductor Material Models](#)
- [Chapter 9, Insulator Material Models](#)
- [Chapter 10, Mobility Models](#)
- [Chapter 11, Scattering Mechanisms](#)
- [Chapter 12, Scattering Models](#)
- [Chapter 13, Binary Alloy Semiconductor Material Models](#)

# 8

## Semiconductor Material Models

---

*This chapter describes the general semiconductor material model as defined and used in Garand.*

For details about default models and parameter values for specific semiconductors, see [Default Semiconductor Materials on page 381](#).

This model applies to both drift-diffusion and Monte Carlo simulations. While only a simpler higher-level description is required for drift-diffusion simulations, all the required parameter values are derived from this more fundamental model. Doing so ensures consistency between drift-diffusion and Monte Carlo simulations. Therefore, the semiconductor material model is the minimum set of parameters required to define a semiconductor for Monte Carlo simulations. As a consequence, some parameters might have no impact on drift-diffusion simulations.

---

### Defining Semiconductor Material Models

This model is a flexible definition that states how the material must be modeled. The definition of the semiconductor material model fundamentally consists of the following separate models:

- The *bulk material model* is common to semiconductors in both drift-diffusion and Monte Carlo simulations (see [Bulk Material Model on page 266](#)).
- The *band structure model* is defined in two parts: a nominal band edge model and a multivalley dispersion model (see [Band Structure Model on page 270](#)).
- The *transport model* is uniquely represented in drift-diffusion simulations by a local equilibrium mobility model definition and is represented in Monte Carlo simulations by a scattering mechanism model definition that is tied to the valley dispersion definition.

## Chapter 8: Semiconductor Material Models

### Bulk Material Model

## Bulk Material Model

The bulk material model is common to semiconductors in both drift-diffusion and Monte Carlo simulations. It consists of a set of bulk material parameters describing the electrical and mechanical properties of a semiconductor material.

Table 28     *Parameters of the bulk material model*

Parameter symbol	Parameter name	Description	Unit
<b>Crystal lattice and orientation in simulation domain</b> (see <a href="#">Crystal Lattice and Orientation</a> )			
$ a $	a	Sets the magnitude of lattice vector $a$ .	Å
$ b $	b	Sets the magnitude of lattice vector $b$ .	Å
$ c $	c	Sets the magnitude of lattice vector $c$ .	Å
$\alpha$	alpha	Sets the angle between $b$ and $c$ .	degree
$\beta$	beta	Sets the angle between $c$ and $a$ .	degree
$\gamma$	gamma	Sets the angle between $a$ and $b$ .	degree
$\langle h k l \rangle_x$	x	Sets the orientation in the x-direction.	—
$\langle h k l \rangle_y$	y	Sets the orientation in the y-direction.	—
$\langle h k l \rangle_z$	z	Sets the orientation in the z-direction.	—
<b>Bulk electrical and mechanical properties</b> (see <a href="#">Bulk Electrical and Mechanical Properties</a> )			
$\kappa$	permittivity	Sets the scalar static dielectric constant.	—
$\kappa_\infty$	k_inf	Sets the high-frequency scalar relative permittivity.	—
$\rho$	density	Sets the mass density of the material.	g/cm <sup>3</sup>
$C_{11}$	C11	Sets a unique elastic stiffness matrix element, assuming cubic symmetry, that models material stress.	GPa

## Chapter 8: Semiconductor Material Models

### Bulk Material Model

Table 28 Parameters of the bulk material model (Continued)

Parameter symbol	Parameter name	Description	Unit
$C_{12}$	$C_{12}$	Sets a unique elastic stiffness matrix element, assuming cubic symmetry, that models material stress.	GPa
$C_{44}$	$C_{44}$	Sets a unique elastic stiffness matrix element, assuming cubic symmetry, that models material stress.	GPa

## Crystal Lattice and Orientation

You define the crystal lattice in terms of the Bravais lattice vectors  $a$ ,  $b$ , and  $c$  that are specified by their magnitudes ( $a$ ,  $b$ , and  $c$ ) and angles ( $\alpha$ ,  $\beta$ , and  $\gamma$ ), which define the orientation of the lattice vectors with respect to one another. The crystal lattice in turn defines the reciprocal lattice vectors by which positions within the first Brillouin zone are referenced.

The crystal lattice orientation is defined with respect to the Cartesian coordinates of the simulation domain by specifying a substrate orientation and a channel orientation as Miller indices, as follows:

- $x \langle h k l \rangle_x$  are the Miller indices that define a direction within the semiconductor crystal. This direction is aligned with the x-axis of the simulation domain.
- $y \langle h k l \rangle_y$  are the Miller indices that define a direction within the semiconductor crystal. This direction is aligned with the y-axis of the simulation domain.
- $z \langle h k l \rangle_z$  are the Miller indices that define a direction within the semiconductor crystal. This direction is aligned with the z-axis of the simulation domain.

#### Note:

These orientations completely orientate the material in the simulation. Because the Miller indices define directions colinear to two orthogonal directions within the simulation domain (for example, the x-axis and z-axis), the Miller indices must themselves be orthogonal. The orientation must be defined using at least two from  $x$ ,  $y$ , and  $z$  (there are default values for each material).

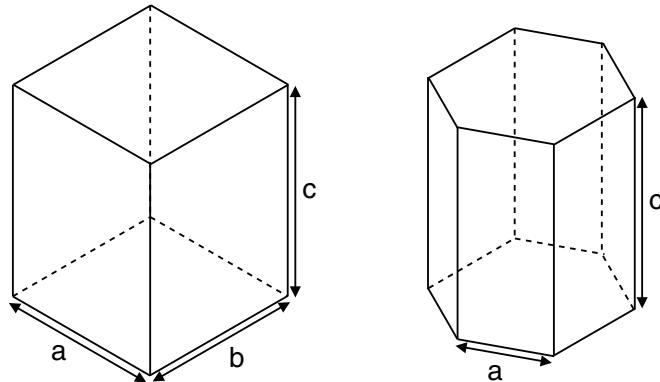
## Defining the Orientation for Cubic Semiconductors

For cubic semiconductors,  $a = b = c$ , and  $\alpha = \beta = \gamma = 90^\circ$  (see [Figure 33 \(left\)](#)). A Cartesian basis is used and this description can be applied in a straightforward way.

## Chapter 8: Semiconductor Material Models

### Bulk Material Model

Figure 33 (Left) Unit cell for cubic lattice and (right) hexagonal lattice system

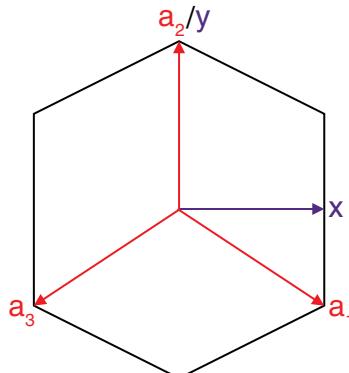


### Defining the Orientation for Hexagonal Semiconductors

For semiconductors with a hexagonal lattice type,  $a = b \neq c$ , and  $\alpha = \beta = 120^\circ$ , and  $\gamma = 90^\circ$  (see Figure 33 (right)). In this case, three axes are defined in the basal plane ( $a_1$ ,  $a_2$ , and  $a_3$  as shown in Figure 34) that are  $120^\circ$  apart, along with a fourth axis,  $c$ , which is at a  $90^\circ$  angle to this plane.

Where a semiconductor with a hexagonal basis is used, a transformation from the hexagonal basis to a Cartesian basis ( $x$ ,  $y$ ,  $z$ ) is performed internally. These axes are illustrated in Figure 34 for the in-plane axes, with the  $c$ -axis and  $z$ -axis aligned.

Figure 34 Axis for the hexagonal basis



In addition, for materials with a hexagonal basis, the following options are available for defining orientations:

- Miller indices of the form  $\langle hkl \rangle$ , where the  $a_1$ -,  $a_2$ -, and  $c$ -axis are considered
- Miller–Bravais indices of the form  $\langle hkil \rangle$ , where the  $a_1$ -,  $a_2$ -,  $a_3$ -, and  $c$ -axis are considered

## Chapter 8: Semiconductor Material Models

### Bulk Material Model

Where the orientation is written to screen, they are represented as Miller indices following conversion to the Cartesian basis.

To convert a four-component Miller–Bravais index  $\langle h k i l \rangle$  to a three-component Miller index  $\langle u v w \rangle$ , the following relations can be used:

$$u = 2h + k$$

$$v = 2k + h$$

$$w = l$$

To perform the reverse conversion:

$$h = \frac{1}{3}(2u - v)$$

$$k = \frac{1}{3}(2v - u)$$

$$i = -(h + k)$$

$$l = w$$

## Changing Default Parameter Values

You can change the default parameter values in the input file by using the following syntax (see [Channel and Substrate Orientations on page 214](#)):

```
material <material>.crystal.<parameter> <value>
```

where:

- `<material>` is the name of a material.
- `<parameter>` is the name of a parameter listed in [Table 28 on page 266](#).
- `<value>` is the new value of the parameter, specified in the expected type.

### Example

Define the substrate and channel orientations of silicon such that the crystallographic (110) planes are normal to the z-axis of the simulation domain and the  $\langle 111 \rangle$  direction is parallel to the x-axis of the simulation domain:

```
material Silicon.crystal.z 1 1 0
material Silicon.crystal.x -1 1 1
```

The substrate and channel directions must be orthogonal.

For a wurtzite material where a hexagonal basis is used, to define the substrate and channel orientations of GaN such that the crystallographic (0001) planes are normal to the z-axis of

## Chapter 8: Semiconductor Material Models

### Band Structure Model

the simulation domain and the  $\langle 10\bar{1}0 \rangle$  direction is parallel to the x-axis of the simulation domain, specify:

```
material GaN.crystal.z 0 0 0 1  
material GaN.crystal.x 1 0 -1 0
```

The substrate and channel directions must be orthogonal following conversion to the Cartesian basis.

---

## Bulk Electrical and Mechanical Properties

The common scalar material parameters for bulk electrical and mechanical properties are listed in [Table 28 on page 266](#).

## Changing Default Parameter Values

You can change the default parameter values in the input file by using the following syntax:

```
aterial <material>.<parameter> <value>
```

where:

- `<material>` is the name of a material.
- `<parameter>` is the name of a parameter listed in [Table 28](#).
- `<value>` is the new value of the parameter, specified in the expected type.

### Example

Redefine the permittivity of silicon and the  $C_{12}$  element of the associated stiffness matrix:

```
material Silicon.permittivity 12.1  
material Silicon.C12 -36.0
```

---

## Band Structure Model

Semiconductor materials define both a conduction band model and a valence band model. Each band is modeled separately and consists of a *band container* that defines the nominal band edge and a list of bands. Each band within the band container defines a dispersion model and a set of valley models with respect to the band edge. These objects, and their parameters, form a hierarchy that is referenced in the input file by the following commands:

```
MATERIAL <material>.<bandcontainer>.<parameter>  
MATERIAL <material>.<bandcontainer>.<band>.<parameter>  
MATERIAL <material>.<bandcontainer>.<band>.<valley>.<parameter>
```

where `bandcontainer` is either `conduction` or `valence`.

## Chapter 8: Semiconductor Material Models

### Band Structure Model

The band container model defines the edge of the list of conduction or valence bands with respect to the vacuum level in the absence of strain. In addition, some specific properties associated with all bands in the container are defined (see [Band Container Model on page 271](#)).

Each band model within the band container defines a set of analytic valleys in the effective mass approximation (EMA) (see [Analytic Multivalley Dispersion Model on page 277](#)). This set of ellipsoidal nonparabolic valleys are distributed within the Brillouin zone and can be used directly to define a multivalley dispersion model for transport, or they can be used to label valleys for scattering within an imported full band structure.

Flexibility in modeling materials is achieved within the band structure model through the number of analytic valleys and their parameter values.

---

## Band Container Model

[Table 29](#) lists the parameters of the band container model, which are conduction band and valence band edge properties.

*Table 29 Parameters of band container model*

Parameter symbol	Parameter name	Description	Unit
$E_0$	E	Sets the energy of the band edge with respect to the vacuum level.	eV
$E_T$	Et	Sets the threshold energy above the dispersion minimum and below which the EMA model is used.	eV
$m_{dg_x}$	dgx	Sets the x-component of the density-gradient effective mass for carriers associated with the band.	$m_e$
$m_{dg_y}$	dgy	Sets the y-component of the density-gradient effective mass for carriers associated with the band.	$m_e$
$m_{dg_z}$	dgz	Sets the z-component of the density-gradient effective mass for carriers associated with the band.	$m_e$

## Nominal Affinity and Band Gap

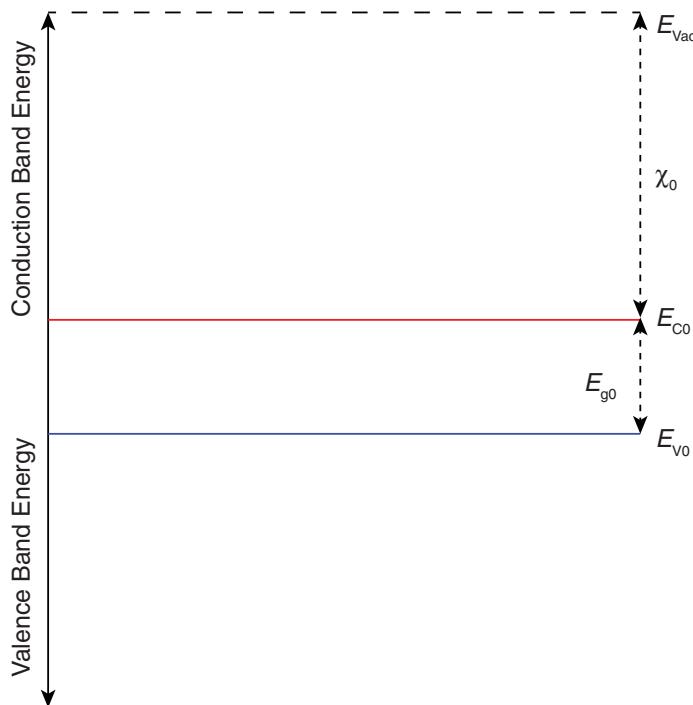
The nominal material affinity and band gap,  $\chi_0$  and  $E_{g0}$ , are not defined directly but are determined from the nominal conduction band and valence band edges,  $E_{C0}$  and  $E_{V0}$ , as illustrated in [Figure 35](#).

## Chapter 8: Semiconductor Material Models

### Band Structure Model

You can modify the affinity and the band gap either directly by specifying nondefault band-edge parameter values or indirectly by the application of strain.

**Figure 35** Typical band model, highlighting the energy reference for the valley minima and both the nominal and actual band edges



## Default Band-Edge Parameter Values

See [Default Semiconductor Materials on page 381](#) for the default band-edge parameter values for each semiconductor material model.

## Changing the Default Band-Edge Parameter Values

To change the default band-edge parameter values in the input file, use the following syntax:

```
material <material>.〈bandcontainer〉.〈parameter〉 <value>
```

where:

- **〈material〉** is the name of a material.
- **〈bandcontainer〉** is either `conduction` or `valence`.
- **〈parameter〉** is the name of a parameter listed in [Table 29](#).
- **〈value〉** is the new value of the parameter, specified in the expected type.

## Chapter 8: Semiconductor Material Models

### Band Structure Model

#### Examples

Define the conduction band and valence band edges of silicon to be 5.0 eV and 5.5 eV, respectively, below the vacuum level:

```
material Silicon.conduction.E 5.00
material Silicon.valence.E      5.50
```

This then defines the electron affinity to be 5.0 eV and the band gap to be 0.5 eV.

Define the x-component of the density-gradient effective mass in the silicon valence band to be 0.47  $m_e$ :

```
material Silicon.valence.dgx 0.47
```

---

## Band Model

The conduction and valence band containers, associated with semiconductors, each define a set of bands. Each band defines a dispersion with respect to the band edge, defined by the parent band container. This dispersion can be a set of analytic valleys or a numeric dispersion read from a file.

Table 30 Parameters of band model

Parameter symbol	Parameter name	Description	Unit
$E$	$E$	Sets the energy of the band with respect to the band edge. This parameter defines the energy of the band with respect to the band edge, which is defined by the band container parameter $E$ with respect to the vacuum level. The final band edge with respect to the vacuum is always defined by the lowest-lying band.	eV
$E_T$	$E_t$	Sets the threshold energy specific to the band (supersedes the band container value). This parameter defines a boundary between numerically tabulated bands and an approximate effective mass model. Below this energy, carrier dynamics are determined by the effective mass model.	eV
Model	model	Specifies the model to use. Options are: <ul style="list-style-type: none"><li>• ema: Use EMA. This is the default.</li><li>• tabulated: Use tabulated dispersion.</li></ul>	—
Path	path	Sets the path to the tabulated band file.	—

## Chapter 8: Semiconductor Material Models

### Band Structure Model

## Defining an EMA Multivalley Model

You can select an analytic effective mass dispersion, using the default analytic valleys defined for a band, by setting the band model parameter as:

```
MATERIAL <material>. <bandcontainer>. <band>.model ema
```

Carrier initialization, propagation within the band, and scattering into the band are then consistent with the multivalley definition.

## Full Band Model

An externally calculated band structure can be associated with a numerically tabulated band and read from a file by setting the following band parameters:

```
MATERIAL <material>. <bandcontainer>. <band>.model tabulated  
MATERIAL <material>. <bandcontainer>. <band>.path <path_to_band_file.dat>
```

Carrier initialization, propagation within the band, and scattering into the band are then consistent with the calculated energy dispersion.

An analytic multivalley model is required to identify the minima within a calculated band, associating a name and scattering mechanisms with them. The position of the analytic valley is mapped to a local minimum in the calculated band, and all mechanisms associated with the named valley are associated with the local minimum. Similarly, all mechanisms scattering into the named valley scatter into the local minimum.

The scattering model might differ when using a tabulated, imported band compared to an analytic band. This can be due to available models or parameters. Parameter sets suitable for use with imported bands are available as part of the Garand MC installation, and you can access them by using the tabulated compatibility command-line option as follows:

```
garand-mc -f <command_file> --compatible tabulated
```

Using this command, all materials that have an available parameter set for tabulated bands are loaded. It is assumed that all materials and bands use a tabulated band-structure, and all parameter sets are loaded consistent with this assumption.

To use a mixture of analytic and tabulated bands within a simulation domain, it might be necessary to include some additional material parameter definitions in the command file.

Imported tabulated band-structure files are preferably in binary format and, by default, it is assumed the  $k$ -vector grid is defined in units of  $(2\pi/a, 2\pi/b, 2\pi/c)$  for semiconductors with a zinc-blende lattice and  $(2\pi/\sqrt{3}a, 4\pi/3b, 2\pi/c)$  for semiconductors with a wurtzite lattice, where  $a$ ,  $b$ , and  $c$  are the lattice constants. This avoids issues where the lattice constants in Garand MC differ from those used when calculating the band structure and allows the mesh to be defined such that it aligns to the edge of the Brillouin zone.

## Chapter 8: Semiconductor Material Models

### Band Structure Model

Prior to Version S-2021.06 of Garand MC, the imported file was assumed to be ASCII text and the  $k$ -vector grid was defined in units of  $\text{\AA}^{-1}$ . Therefore, it was required that the lattice constant used in Garand MC matched that used in the band-structure calculation to avoid inconsistencies in the definition of the  $k$ -vector grid that might lead to unstable or incorrect simulations.

For backward compatibility, when an ASCII (formatted) band-structure file is read in, the  $k$ -vector grid is assumed to be in units of  $\text{\AA}^{-1}$  and, when a binary (unformatted) band-structure file is read in, the  $k$ -vector grid is assumed to be in units as previously defined.

This default behavior can be overwritten. To set the grid in units of  $\text{\AA}^{-1}$ , specify:

```
material <material>.bandcontainer.<band>.k_vector_unit A
```

You can also set the grid in units of  $2\pi/a$  by specifying:

```
material <material>.bandcontainer.<band>.k_vector_unit 2pia
```

When ASCII files are read in, the simulator tries to align the lattice constants to improve the stability of the simulation. This assumes that the tabulation of the band structure runs to  $2\pi/a$ . If this is not the case or this alignment is not required, then you can deactivate the feature by using the following command:

```
material <material>.crystal.align_lattice_constant off
```

#### Note:

This command is included primarily for backward compatibility purposes and should be used with caution to avoid inaccurate or unstable simulations.

---

## Selecting the Transport Model

By default, the effective density-of-states (DOS) is defined in both drift-diffusion and Monte Carlo simulations by using the analytic multivalley model with masses stored in the Garand material database.

To calculate the DOS for the valence band using the six-band  $k \cdot p$  band structure model, specify the following commands:

```
material <material>.valence.kp_dos on  
material <material>.valence.fullband on
```

The first command ensures that the necessary parameters are updated, and the second command activates the  $k \cdot p$  calculations required. A spherical average of the effective mass for each valley included in the valence model is extracted as thermal energy and then is used to calculate the effective DOS, accounting for the impact of applied stress.

## Chapter 8: Semiconductor Material Models

### Band Structure Model

For the conduction band, either of the following band structures can be used for electron transport:

- Analytic multivalley model (which is the default)
- Numerically tabulated band with values read from a file

To select the analytic multivalley model, use the following syntax:

```
material <material>.conduction.<band>.model ema
```

To select the numerically tabulated band, along with the path to the file, specify:

```
material <material>.conduction.<band>.model tabulated  
material <material>.conduction.<band>.path <path_to_band_file.dat>
```

For most materials, the six-band  $k \cdot p$  model is used for hole transport in Garand MC. This model involves the precalculation and tabulation of various parameters providing accuracy but with an additional computational overhead (see [Storing  \$k \cdot p\$  Band Structures on page 225](#)). In addition to this, the EMA and numerically tabulated models described here can be used for hole transport.

To select the tabulated  $k \cdot p$  band-structure model, use the following syntax:

```
material <material>.valence.<band>.model 6kp
```

To select the numerically tabulated band, along with the path to the file, specify:

```
material <material>.valence.<band>.model tabulated  
material <material>.valence.<band>.path <path_to_band_file.dat>
```

To use the analytic model using EMA to determine hole transport, the syntax is:

```
material <material>.valence.<band>.model ema
```

This model sacrifices some of the accuracy of the  $k \cdot p$  approach, particularly at high fields, but it has the benefit of reducing the computational overhead, allowing for shorter simulation times. The default effective masses used for the analytic transport model for holes can be redefined in the input file in one of the following ways:

- Overwrite the default effective masses as described in [Nonparabolic Dispersion Relation on page 293](#). This results in the same masses being used for both the DOS and transport.
- Define distinct transport masses that will be used only for propagation and scattering, but not the effective DOS. This is similar to the case of activating the  $k \cdot p$  model for transport but not for the DOS calculation.
- Extract transport masses from a  $k \cdot p$  calculation at a given energy relative to the valley minima.

## Chapter 8: Semiconductor Material Models

### Band Structure Model

The parameter names used to define the transport mass are given in [Band Structure Model on page 270](#). It might be necessary to redefine the axis orientation of the valley consistent with the device orientation. To extract the transport effective mass from the  $k \cdot p$  calculation, specify the following commands:

```
material <material>.valence.transport_mass fullband_6kp  
material <material>.valence.fullband on
```

The orientation of the valleys is updated automatically to match the device orientation in this case. By default, this mass is extracted at the valley minima, but an offset measured from the minima in eV can be introduced by setting:

```
material <material>.valence.transport_mass_energy <float>
```

---

## Analytic Multivalley Dispersion Model

You can model band dispersion using a set of generalized analytic, singly degenerate, ellipsoidal, nonparabolic valleys [1] (see [Analytic Valley Model on page 293](#)). The nominal band edge defines the reference energy from which each valley minima is defined (see [Band Container Model on page 271](#)). Each valley within a material band model can be referenced by its name, which is unique in the set of valleys within the same band model.

### Analytic Valley Parameters

[Table 31](#) lists the analytic, singly degenerate, ellipsoidal, nonparabolic valley parameters.

*Table 31 Valley model parameters*

Parameter symbol	Parameter name	Description	Unit
<b>Valley position and orientation in crystal lattice</b>			
$k_0$	pos	Sets the position of the valley minima within the first Brillouin zone as a vector, where the vector basis is the crystal reciprocal lattice vectors, where: <ul style="list-style-type: none"><li>• <math>k = (0, 0, 0)</math> denotes the zone center.</li><li>• <math>k = (1, 0, 0)</math> denotes the <math>X</math>-symmetry points.</li><li>• <math>k = (1/2, 1/2, 1/2)</math> denotes the <math>L</math>-symmetry points.</li></ul>	$2\pi(1/a, 1/b, 1/c)$
x-axis	x	Sets the orientation of the <i>longitudinal</i> axis of the valley within the first Brillouin zone as a set of Miller indices.	$\langle hkl \rangle$

## Chapter 8: Semiconductor Material Models

### Band Structure Model

Table 31 Valley model parameters (Continued)

Parameter symbol	Parameter name	Description	Unit
y-axis	y	Sets the orientation of the <i>transverse</i> axis of the valley within the first Brillouin zone as a set of Miller indices.	<hkl>
z-axis	z	Sets the orientation of the <i>transverse</i> axis of the valley within the first Brillouin zone as a set of Miller indices.	<hkl>
<b>Valley parameters</b>			
$\Delta E$	E	Sets the energy of the valley minima with reference to the nominal band edge. Positive values represent valley minima that require higher carrier energy.	eV
$\delta E$	dE	Sets a shift in energy of the valley minima with reference to the nominal band edge, applied in addition to any shift due to strain. Positive values represent valley minima that require higher carrier energy.	eV
$m_x$	mx	Sets the <i>longitudinal</i> effective mass (aligning the longitudinal axis with the Cartesian x-axis).	$m_e$
$m_y$	my	Sets the <i>transverse</i> effective mass (aligning the transverse axis with the Cartesian y-axis).	$m_e$
$m_z$	mz	Sets the <i>transverse</i> effective mass (aligning the transverse axis with the Cartesian z-axis).	$m_e$
$m_{qx}$	mqx	Sets the confinement effective mass along the x-axis of the device. This is set automatically based on the crystal orientation, but it can be changed to suit the user specification.	$m_e$
$m_{qy}$	mqy	Sets the confinement effective mass along the y-axis of the device. This is set automatically based on the crystal orientation, but it can be changed to suit the user specification.	$m_e$
$m_{qz}$	mqz	Sets the confinement effective mass along the z-axis of the device. This is set automatically based on the crystal orientation, but it can be changed to suit the user specification.	$m_e$

## Chapter 8: Semiconductor Material Models

### Band Structure Model

Table 31 Valley model parameters (Continued)

Parameter symbol	Parameter name	Description	Unit
$m_{tx}$	mtx	Sets the longitudinal transport effective mass. It applies only to hole transport.	$m_e$
$m_{ty}$	mtv	Sets the transverse transport effective mass. It applies only to hole transport.	$m_e$
$m_{tz}$	mtz	Sets the transverse transport effective mass. It applies only to hole transport.	$m_e$
$\alpha$	alpha	Sets the valley nonparabolicity factor.	—
$Z_f$	zf	Sets the fraction of the valley to be considered within the first Brillouin zone. This distinguishes valleys with minima located within the first Brillouin zone ( $Z_f = 1.0$ ) from those with minima located at the zone boundary ( $Z_f = 0.5$ ).	—
<b>Strain deformation</b>			
$\Xi_u$	xi_u	Sets the uniaxial deformation potential.	eV
$\Xi_d$	xi_d	Sets the dilatation deformation potential.	eV
$\Xi'_u$	xi_u_prime	Sets the deformation potential for splitting the two lowest conduction bands at the zone edge. It is used when calculating the electron effective mass under the influence of strain.	eV
$\delta$	delta	Sets the size of the split (separation) of the two lowest conduction bands at the zone edge. It is used when calculating the electron effective mass under the influence of strain.	eV
$M$	M	Sets a fitting parameter for electron mass.	—

## Default Analytic Valley Parameters

See [Default Semiconductor Materials on page 381](#) for the default analytic valley parameter values for each semiconductor material model.

## Changing Default Analytic Valley Parameter Values

This section describes how to change the default parameter values.

### Valley Position and Orientation

To change the default values of the valley position and orientation parameters in the input file, use the following syntax:

```
material <material>.<bandcontainer>.<band>.<valley>.min.<parameter>
<value>
```

where:

- <material> is the name of a material.
- <bandcontainer> is either conduction or valence.
- <band> is the name of a band in the band container.
- <valley> is the name that identifies the valley minimum.
- min denotes the specification of a valley position or orientation parameter as given by the name of a parameter (<parameter>) listed in [Table 31 on page 277](#).
- <value> is the new value of the parameter, specified in the expected type.

The following commands define the position of the X1 valley minimum within the first conduction band of silicon to be located at (0.0, 0.0, -0.85), as measured from the zone center to the zone edge, and with an orientation such that the longitudinal axis aligns with the crystallographic reciprocal z-axes:

```
material Silicon.conduction.C1.X1.min.pos  0.0  0.0 -0.85
material Silicon.conduction.C1.X1.min.x    0.0  0.0 -1.0
material Silicon.conduction.C1.X1.min.y   -1.0  0.0  0.0
material Silicon.conduction.C1.X1.min.z    0.0 -1.0  0.0
```

In all cases, the vector basis is the crystallographic reciprocal vectors.

### Valley Parameters

To change the default values of the valley parameters in the input file, use the following syntax:

```
material <material>.<bandcontainer>.<band>.<valley>.<parameter> <value>
```

where:

- <material> is the name of a material.
- <bandcontainer> is either conduction or valence.
- <band> is the name of a band in the band container.

## Chapter 8: Semiconductor Material Models

### Band Structure Model

- `<valley>` is the name that identifies the valley minima.
- `<parameter>` is the name of a valley parameter listed in [Table 31 on page 277](#).
- `<value>` is the new value of the parameter, specified in the expected type.

The following commands define the energy of the X1 valley minimum within the first conduction band of silicon to be a value 0.1 eV below the nominal conduction band edge and defines the effective masses in the x-, y-, and z-axes of the valley to be 0.85, 0.45, and 0.30  $m_e$ , respectively:

```
material Silicon.conduction.C1.X1.E -0.10
material Silicon.conduction.C1.X1.mx 0.85
material Silicon.conduction.C1.X1.my 0.45
material Silicon.conduction.C1.X1.mz 0.30
```

---

## Affinity and Band Gap

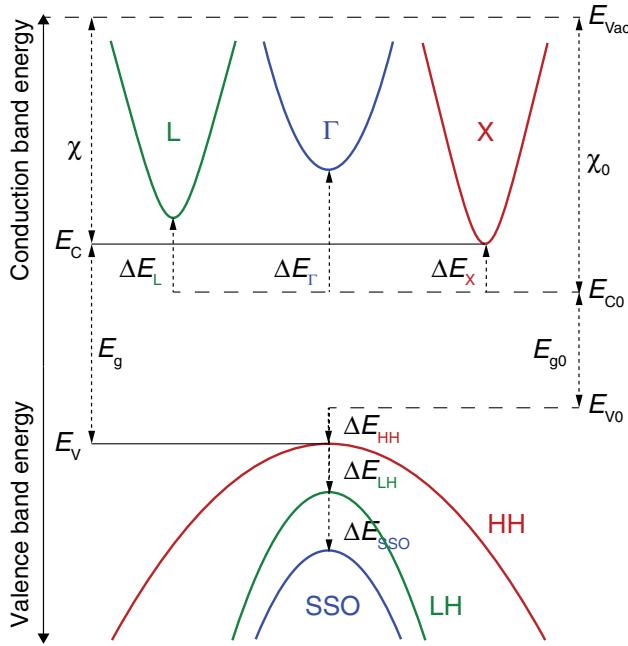
The multivalley model (see [Analytic Multivalley Dispersion Model on page 277](#)) defines the valley minima energy with respect to the edge of the band it is associated with, itself defined with reference to the nominal band edge defined by the band container (see [Band Structure Model on page 270](#)). The lowest-lying minima associated with the conduction band and valence band define the actual conduction and valence band edges,  $E_C$  and  $E_V$ , with respect to the vacuum. This in turn defines the actual simulated band gap  $E_g$  and electron affinity  $\chi$ . Nondefault valley minima energies can be specified such that  $E_C$  and  $E_V$  do not have their nominal band values  $E_{C0}$  and  $E_{V0}$  (see [Changing Default Analytic Valley Parameter Values on page 280](#)).

Similarly, the application of strain adjusts the valley positions and, in doing so, automatically reflects the change in the band gap and affinity from their nominal values  $E_{g0}$  and  $\chi_0$ . [Figure 36](#) illustrates the difference between the nominal and simulated affinity and band gap, following the modification of valley minima energies.

## Chapter 8: Semiconductor Material Models

### Band Structure Model

**Figure 36** Illustration of band model, highlighting the energy reference for the valley minima and both the nominal and actual band edges



### Six-Band $k \cdot p$ Model Definition

The semiconductor valence band dispersion can be defined by a six-band  $k \cdot p$  model (see [Six-Band  \$k \cdot p\$  Model Parameters on page 298](#)). A six-band  $k \cdot p$  model allows for the inclusion of spin-orbit coupling and leads to three numeric valence band solutions throughout the Brillouin zone, referred to as the heavy-hole (HH) band, the light-hole (LH) band, and the spin split-off (SSO) band. Such a model provides an accurate representation of hole transport that is difficult to obtain with an analytic EMA multivalley model due to the complicated anisotropic warped nature of valence bands.

The HH, LH, and SSO solutions are additionally represented by an equivalent analytic valley model that is defined to match the six-band  $k \cdot p$  DOS (see [Analytic Valley Model on page 293](#)). The DOS per band is defined using a spherically averaged effective mass and is required for determining the effective valence band DOS and the intrinsic carrier concentration within Garand. Doing so maintains consistency between Garand and Garand MC. By default, hole transport in Monte Carlo simulations is considered in the six-band  $k \cdot p$  dispersion model.

[Table 32](#) lists the parameters used to define the six-band  $k \cdot p$  band structure model. These parameters define the interaction Hamiltonians for the band structure model.

## Chapter 8: Semiconductor Material Models

### Band Structure Model

Table 32 Parameters of valence band  $k \cdot p$  model

Parameter symbol	Parameter name	Description	Unit
<b>Band properties</b>			
$E_0$	E	Sets the energy of the band edge relative to the vacuum level.	eV
<b>Six-band <math>k \cdot p</math> band structure model</b>			
$L$	L-kp	Sets the $L$ parameter of the model.	$\hbar^2/2m_0$
$M$	M-kp	Sets the $M$ parameter of the model.	$\hbar^2/2m_0$
$N$	N-kp	Sets the $N$ parameter of the model.	$\hbar^2/2m_0$
$l$	l-defpot	Sets the strain deformation potential used to determine the effect of the application of strain.	eV
$m$	m-defpot	Sets the strain deformation potential used to determine the effect of the application of strain.	eV
$n$	n-defpot	Sets the strain deformation potential used to determine the effect of the application of strain.	eV
$\Delta_{so}$	dsso	Sets the spin split-off energy separation.	eV

### Default Six-Band $k \cdot p$ Band Structure Parameters

See [Default Semiconductor Materials on page 381](#) for the default six-band  $k \cdot p$  parameter values for each semiconductor material model.

## Changing the Default Six-Band k·p Parameter Values

To change the default values for the six-band k·p parameters in the input file, use the following syntax:

```
material <material>.valence.<parameter> <value>
```

where:

- <material> is the name of a material.
- <parameter> is the name of a parameter listed in [Table 32 on page 283](#).
- <value> is the new value of the parameter, specified in the expected type.

### Example

Define the density-gradient effective x-mass as  $0.25 m_e$ , the  $L$  parameter as  $-6.10 \hbar^2 / 2m_e$ , and the  $n$  deformation potential as -10.0 eV:

```
material Silicon.valence.dgx      0.25
material Silicon.valence.L-kp     -6.10
material Silicon.valence.n-defpot -10.0
```

## Full Band Model

You can use a numerically tabulated band for both electron and hole transport, with values read from a file created using an external band-structure calculation.

To define the path to the file, specify the following in the command file:

```
material <material>.<bandlist>.<band>.path <path_to_band_file.dat>
```

An unstressed silicon band-structure is supplied by default with the installation of Garand, and the files are located in the following location:

```
$STROOT/tcad/current/linux64/lib/GARAND/materials/
```

To use these band-structure files, use the following commands in the input file, where <path> is the location of the band-structure files as previously provided:

```
MATERIAL Silicon.conduction.C1.model tabulated
MATERIAL Silicon.conduction.C1.path  <path>/SiGe_xGe0.0_band_10.dat

MATERIAL Silicon.conduction.C2.model tabulated
MATERIAL Silicon.conduction.C2.path  <path>/SiGe_xGe0.0_band_12.dat

MATERIAL Silicon.valence.HH.model tabulated
MATERIAL Silicon.valence.HH.path   <path>/SiGe_xGe0.0_band_8.dat

MATERIAL Silicon.valence.LH.model tabulated
MATERIAL Silicon.valence.LH.path   <path>/SiGe_xGe0.0_band_6.dat
```

## Chapter 8: Semiconductor Material Models

### Material Strain

```
MATERIAL Silicon.valence.SSO.model tabulated
MATERIAL Silicon.valence.SSO.path <path>/SiGe_xGe0.0_band_4.dat
```

To ensure the correct scattering models and parameters are applied, use the `-c` tabulated command-line option.

---

## Material Strain

You apply strain to a material using biaxial or uniaxial statements in the input file.

---

### Biaxial Strain

You apply biaxial strain to semiconductor layers using a relaxed substrate material, which has the following effects [2]:

- Band edges shift, with some usually degenerate bands splitting.
- The bands themselves warp, resulting in a change of effective mass (both conductivity and DOS), which influences transport and scattering.

The longitudinal strain is defined based on the lattice constant of the layer to be strained and the relaxed substrate:

$$\epsilon_{\parallel} = \frac{a_{\text{layer}} - a_{\text{substrate}}}{a_{\text{substrate}}} \quad (77)$$

The normal strain is:

$$\epsilon_{\perp} = -\nu \epsilon_{\parallel} \quad (78)$$

where  $\nu$  is the Poisson ratio, which is defined based on the substrate orientation from the elastic constants  $C_{11}$ ,  $C_{12}$ , and  $C_{44}$ . In-plane strain can be applied to three principal material substrate orientations: (001), (110), and (111).

For the (001) substrate orientation, the elements of the strain tensor are given by [3][4]:

$$\epsilon_{xx} = \epsilon_{yy} = \epsilon_{\parallel} \quad (79)$$

$$\epsilon_{zz} = \epsilon_{\perp} \quad (80)$$

$$\nu = \frac{2C_{12}}{C_{11}} \quad (81)$$

For the (110) substrate orientation:

$$\epsilon_{xx} = \epsilon_{yy} = \frac{1}{2}(\epsilon_{\perp} + \epsilon_{\parallel}) \quad (82)$$

$$\epsilon_{zz} = \epsilon_{\parallel} \quad (83)$$

## Chapter 8: Semiconductor Material Models

### Material Strain

$$\epsilon_{xy} = \frac{1}{2}(\epsilon_{\perp} - \epsilon_{\parallel}) \quad (84)$$

$$\nu = \frac{C_{11} + 3C_{12} - 2C_{44}}{C_{11} + C_{12} + 2C_{44}} \quad (85)$$

For the (111) substrate orientation:

$$\epsilon_{xx} = \epsilon_{yy} = \epsilon_{zz} = \frac{1}{3}(\epsilon_{\perp} + 2\epsilon_{\parallel}) \quad (86)$$

$$\epsilon_{xy} = \epsilon_{xz} = \epsilon_{yz} = \frac{1}{3}(\epsilon_{\perp} - \epsilon_{\parallel}) \quad (87)$$

$$\nu = \frac{2C_{11} + 4C_{12} - 4C_{44}}{C_{11} + 2C_{12} + 4C_{44}} \quad (88)$$

The unspecified elements are zero and, due to symmetry,  $\epsilon_{ij} = \epsilon_{ji}$ .

## Input File Commands

Biaxial strain from a relaxed buffer layer can be defined in different ways. The lattice constant of the buffer layer can be specified in ångströms, or a percentage change can be defined.

*Table 33 Parameters for biaxial strain*

Parameter	Description	Type	Default	Unit
a	Sets the lattice constant of the material, where $a > 0.0$ .	float	–	Å
orient	Sets the surface orientation.	vector	–	–
per	Sets the level of strain as a percentage, where $ per  > 0.0$	float	0.0	%

### Examples

Strain germanium by the lattice constant of silicon:

```
strain Germanium.biaxial.a 5.43
```

Define the level of strain as a percentage, where the magnitude is signed negative for compressive strain and signed positive for tensile strain:

```
strain Germanium.biaxial.per -1.0
```

By default, it is applied to whichever substrate orientation is defined for the material in question, but this can be altered in the input file. For example:

```
strain Germanium.biaxial.orient 0 0 1
```

## Uniaxial Stress

To apply uniaxial stress along the direction  $\langle hkl \rangle$ , you first choose a coordinate system where the stress of magnitude  $P$  (in GPa) is applied to the [001] direction, giving a stress tensor of the form [5]:

$$\sigma' = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & P \end{bmatrix} \quad (89)$$

This initial tensor can be translated to the  $\langle hkl \rangle$  direction to give the final stress tensor.

The strain tensor can be derived from:

$$\begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ 2\epsilon_{yz} \\ 2\epsilon_{xz} \\ 2\epsilon_{xy} \end{bmatrix} = s \begin{bmatrix} s_{11} & s_{12} & s_{12} & 0 & 0 & 0 \\ s_{12} & s_{11} & s_{12} & 0 & 0 & 0 \\ s_{12} & s_{12} & s_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & s_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & s_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & s_{44} \end{bmatrix} \begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{bmatrix} \quad (90)$$

The compliance constants are given by:

$$\begin{aligned} s_{11} &= \frac{C_{11} + C_{12}}{C_{11}^2 + C_{11}C_{12} - 2C_{12}^2} \\ s_{12} &= \frac{-C_{12}}{C_{11}^2 + C_{11}C_{12} - 2C_{12}^2} \\ s_{44} &= \frac{1}{C_{44}} \end{aligned} \quad (91)$$

## Input File Commands

To introduce uniaxial strain to the system, you specify two values:

- The first value is a scalar describing the type of strain (negative for compressive and positive for tensile) and magnitude in GPa.
- The second value is a direction along which the strain is applied.

## Chapter 8: Semiconductor Material Models

### Material Strain

Table 34 Parameters for uniaxial strain

Parameter	Description	Type	Default	Unit
orient	Sets the direction of the applied strain.	vector	–	–
P	Sets the applied strain, where $ P  > 0.0$ . By default, no strain is applied. If no direction is specified for uniaxial strain, then the strain applies along the channel direction.	float	0.0	GPa

### Example

Introduce 1 GPa compressive strain along the [110] direction:

```
strain Germanium.uniaxial.P      -1.0
strain Germanium.uniaxial.orient  1 1 0
```

The definition of the orientation is the same as that used to define substrate and channel orientations.

---

## Other strain Commands

This section describes other specifications available using the `strain` command.

### Specifying Tensors

Stress or strain tensors can be defined in the input file in either the crystal or device frame of reference. Only one tensor of either type can be defined for any given material.

As with individual uniaxial sources, stress is defined in units of GPa, with tensile stress given as positive and compressive stress given as negative.

To define a strain tensor in the crystal frame, specify:

```
strain <material>.crystal_strain_tensor εxx, εyy, εzz, εyz, εxz, εxy
```

To define a stress tensor in the crystal frame, specify:

```
strain <material>.crystal_stress_tensor σxx, σyy, σzz, σyz, σxz, σxy
```

To define a strain tensor in the device frame, specify:

```
strain <material>.device_strain_tensor εxx, εyy, εzz, εyz, εxz, εxy
```

To define a stress tensor in the device frame, specify:

```
strain <material>.device_stress_tensor σxx, σyy, σzz, σyz, σxz, σxy
```

## Specifying Multiple Strain Definitions

If multiple strain definitions are required for a given material, you must modify the syntax to give each definition a unique identifier:

```
strain <material>.<type>.<name>.<parameter> value
```

**Note:**

For multiple strain definitions, the name applied to each definition must be unique to avoid ambiguous behavior.

For example:

```
strain Silicon.uniaxial.str1.P      0.5
strain Silicon.uniaxial.str1.orient 1 1 0
strain Silicon.uniaxial.str2.P      -1.25
strain Silicon.uniaxial.str2.orient 0 0 1
```

If names are not specified, an error is returned with information about how to modify the syntax.

## Controlling Strain Modification

You can control the impact of strain on the band structure by using different parameters.

The shifting of valleys is switched on by default, but can be deactivated by using:

```
material <material>.<bandcontainer>.strain_valleys off
```

Additional shifting from shear stress can also be deactivated independently (it is included by default) by using:

```
material <material>.<bandcontainer>.include_shear_stress off
```

The variation of the effective mass due to stress is switched off by default, but it can be included by using:

```
material <material>.<bandcontainer>.strain_mass on
```

This allows you to modify the electron effective mass for both the electrostatics and transport, and the hole mass for electrostatics only (the impact on transport comes from  $k \cdot p$ ).

---

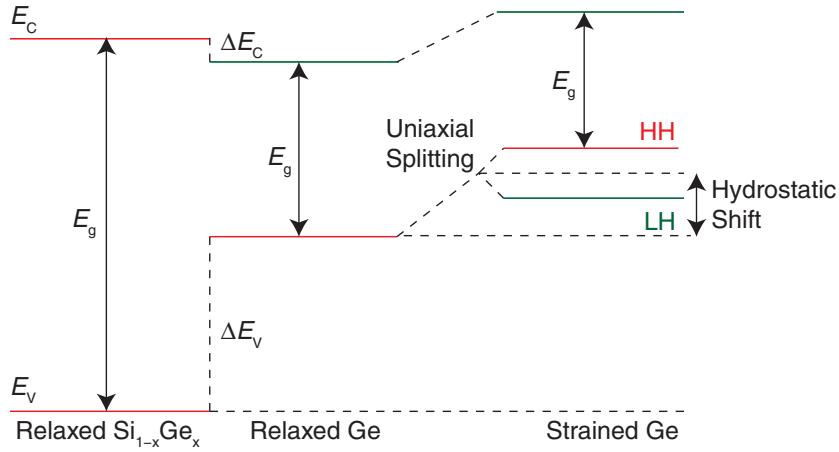
## Strain-Induced Energy Shifts

From linear deformation-potential theory, the strain-induced shifts of conduction bands can be obtained from the above strain tensors (see [Figure 37](#)).

## Chapter 8: Semiconductor Material Models

### Material Strain

**Figure 37** Shift of conduction band and valence band edges in Ge due to compressive biaxial strain induced by a SiGe buffer layer; the shifting of valleys in conduction band depends on both the substrate orientation and the level of strain applied



**Table 35** Energy shifts for conduction bands and L-valleys

Valley orientation	Energy shift
<b>Conduction bands along the <math>\Delta</math> symmetry line [3]</b>	
[100]	$\frac{2}{3}\Xi_u^\Delta \epsilon_{xx} - \frac{1}{3}\Xi_u^\Delta (\epsilon_{yy} + \epsilon_{zz})$
[010]	$\frac{2}{3}\Xi_u^\Delta \epsilon_{yy} - \frac{1}{3}\Xi_u^\Delta (\epsilon_{xx} + \epsilon_{zz})$
[001]	$\frac{2}{3}\Xi_u^\Delta \epsilon_{zz} - \frac{1}{3}\Xi_u^\Delta (\epsilon_{xx} + \epsilon_{yy})$
<b>L-valleys</b>	
[111]	$\frac{2}{3}\Xi_u^L (\epsilon_{xy} + \epsilon_{xz} + \epsilon_{yz})$
[ $\bar{1}$ 11]	$\frac{2}{3}\Xi_u^L (-\epsilon_{xy} - \epsilon_{xz} + \epsilon_{yz})$
[ $\bar{1}$ $\bar{1}$ 1]	$\frac{2}{3}\Xi_u^L (\epsilon_{xy} - \epsilon_{xz} - \epsilon_{yz})$
[1 $\bar{1}$ 1]	$\frac{2}{3}\Xi_u^L (-\epsilon_{xy} + \epsilon_{xz} - \epsilon_{yz})$

## Chapter 8: Semiconductor Material Models

### Material Strain

The hydrostatic component is:

$$\Delta E_C^i = \left( \Xi_d^i + \frac{\Xi_u^i}{3} \right) (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) \quad (92)$$

where  $i$  indicates the shift for X- ( $\Delta$ ) or L-valleys. In [Equation 92](#),  $\Xi_u$  and  $\Xi_d$  are the deformation potentials describing the splitting and hydrostatic components, respectively.

The shift of the valence bands is accounted for by the relevant Hamiltonian, given in [Equation 121 on page 299](#). Uniaxial splitting is given by the  $k \cdot p$  calculation, while the hydrostatic shift for the valence band is given by:

$$\Delta E_v = a_v (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) \quad (93)$$

Here,  $a$  is the hydrostatic deformation potential for the valence band, calibrated to match available experimental data.

An additional shift in energy between the  $\Delta_2$  and  $\Delta_4$  valleys from shear stress components is calculated from [\[6\]](#):

$$\Delta E_{\text{shear}} = \begin{cases} -\Delta \eta^2 / 4 & |\eta| \leq 1 \\ -(2|\eta| - 1)\Delta / 4 & |\eta| > 1 \end{cases} \quad (94)$$

where  $\eta$  is a dimensionless parameter given by:

$$\eta = \frac{4\varepsilon_{xy}\Xi'_u}{\Delta} \quad (95)$$

Here,  $\Delta$  is the separation between the lowest conduction bands at the band edge for the unstrained lattice, and  $\Xi'_u$  is the deformation potential describing the splitting of the lowest conduction bands at the zone boundary:

$$\Delta E = 4\Xi'_u \varepsilon_{xy} \quad (96)$$

The additional shift in energy ( $\Delta E_{\text{shear}}$ ) is added to the other components previously defined.

## Effective Mass

For holes, the effective masses are modified using the  $k \cdot p$  calculation. For electrons, the masses in the  $\Delta$ -valleys of the conduction band are modified using a model that matches well with full band-structure calculations.

## Chapter 8: Semiconductor Material Models

### Nondefault Material Model Definitions

In this case, the masses of the  $\Delta_2$  valleys change, following the approach in [6]:

$$\frac{m_t}{m_{t1}(\eta)} = \begin{cases} \left(1 - \frac{\eta}{M}\right) & |\eta| \leq 1 \\ \left(1 - \frac{\text{sign}(\eta)}{M}\right) & |\eta| > 1 \end{cases} \quad (97)$$

$$\frac{m_t}{m_{t2}(\eta)} = \begin{cases} \left(1 + \frac{\eta}{M}\right) & |\eta| \leq 1 \\ \left(1 + \frac{\text{sign}(\eta)}{M}\right) & |\eta| > 1 \end{cases} \quad (98)$$

$$\frac{m_l}{m_l(\eta)} = \begin{cases} \left(1 - \eta^2\right)^{-1} & |\eta| \leq 1 \\ \left(1 - \frac{1}{\eta}\right)^{-1} & |\eta| > 1 \end{cases} \quad (99)$$

where  $\eta$  is as given in [Equation 95](#), and  $M$  is a fitting parameter.

---

## Nondefault Material Model Definitions

You can change the semiconductor material model definition by specifying not only nondefault model parameter values, but also nondefault model definitions. This is achieved by adding or removing valleys from the material band model (or scattering mechanisms from the valley model).

---

### Removing a Valley Model

To remove defined valleys that are currently included in a band model, use the following syntax:

```
material <material>. <bandcontainer>. <band>. <valley> REMOVE
```

Doing so removes the valley from the band, which affects the DOS, and thereby the intrinsic carrier concentration and scattering rates.

---

### Adding a Valley Model

To add defined valleys that are currently not included in a band model, as a result of being removed, use the following syntax:

```
material <material>. <bandcontainer>. <band>. <valley> ADD
```

## Chapter 8: Semiconductor Material Models

### Analytic Valley Model

Doing so reintroduces the previously defined valley into the band model, which affects the DOS, and thereby the intrinsic carrier concentration and scattering rates.

---

## Analytic Valley Model

Analytic valleys are the basic building block of the analytic conduction band and valence band models. The analytic valley model is described by a generalized degenerate, ellipsoidal nonparabolic model [1].

---

### General Properties

This section discusses the general properties of the model.

### Nonparabolic Dispersion Relation

For a given valley, a state with wavevector  $\mathbf{k} = (k_x, k_y, k_z)$  relative to the wavevector of the valley minima  $\mathbf{k}_0 = (k_{0x}, k_{0y}, k_{0z})$  has energy  $\varepsilon(\mathbf{k})$  above the valley energy minima satisfying:

$$\varepsilon(\mathbf{k})(1 + \alpha\varepsilon(\mathbf{k})) = \Gamma(\mathbf{k}) = \frac{\hbar^2}{2} \left( \frac{k_x^2}{m_x^*} + \frac{k_y^2}{m_y^*} + \frac{k_z^2}{m_z^*} \right) \quad (100)$$

This describes a single valley with three principal axes and an effective mass defined along each. Typically, valleys are defined through their longitudinal and transverse effective masses as valleys exhibit rotational symmetry about the longitudinal axes at energies near the valley minimum. While alignment of the longitudinal axis with respect to the reciprocal lattice vectors generally differs for each valley, the effective masses here are always defined assuming a longitudinal axis aligned to the x-axis of the reciprocal lattice vectors. Therefore,  $m_x^*$  equates to the longitudinal effective mass, and  $m_y^*$  and  $m_z^*$  equate to the mutually perpendicular transverse effective masses.

### Position and Orientation

The position of the valley minima  $\mathbf{k}_0 = (k_{0x}, k_{0y}, k_{0z})$  is specified relative to the Brillouin zone center as fractions of the reciprocal lattice vectors, such that  $(0, 0, 0)$  is the zone center. The valley orientation is defined through the orientation of the longitudinal and transverse axes using Miller indices with respect to the reciprocal lattice vectors. The position and orientation completely specify the relative geometry of multiple valleys.

## Chapter 8: Semiconductor Material Models

### Analytic Valley Model

## Energy Minima

Each valley defines the energy of the valley minima as the difference in energy between the minima and the nominal band edge:

$$\Delta E = E_{\min} - E_0 \quad (101)$$

You can adjust the energy minima through this difference, with increased positive  $\Delta E$  shifting both conduction and valence valley minima to higher energies.

The total energy  $E$  of the state  $\mathbf{k} = (k_x, k_y, k_z)$  is given by the energy minima together with the valley dispersion as follows:

$$E = E_0 + \Delta E + \varepsilon(\mathbf{k}) = E_{\min} + \varepsilon(\mathbf{k}) \quad (102)$$

## Density-of-States

The band model directly determines the DOS. For a general degenerate, ellipsoidal nonparabolic valley, defined by [Equation 100 on page 293](#), the DOS with energy  $\varepsilon$ , relative to the valley minima, is given by:

$$g'(\varepsilon) = \frac{Z}{\pi^2 \hbar^3} m^* \sqrt{2m^* \varepsilon (1 + \alpha\varepsilon)} (1 + 2\alpha\varepsilon) \quad (103)$$

where a factor of 2 accounting for spin degeneracy is included and where the DOS effective mass  $m^*$  has been defined as:

$$m^* = (m_x^* m_y^* m_z^*)^{\frac{1}{3}} \quad (104)$$

By taking a geometric average of the effective masses, the DOS effective mass allows the DOS to be calculated as though the valley had spherically symmetric equienergy surfaces.

Relative to the reference energy level from which the valley minima are measured, the DOS for the general degenerate  $i^{\text{th}}$  valley, with energy minima  $E_i$ , is given by:

$$g_i(E) = \begin{cases} g'(E - E_i) & E \geq E_i \\ 0 & \text{Otherwise} \end{cases} \quad (105)$$

For a given band model comprising a set of degenerate ellipsoidal nonparabolic valleys defined by [Equation 100 on page 293](#), the total DOS is given by:

$$g(E) = \sum_i g_i(E) \quad (106)$$

where  $g_i(E)$  is the single valley DOS, given by [Equation 105](#), for the  $i^{\text{th}}$  valley.

## Chapter 8: Semiconductor Material Models

### Analytic Valley Model

## Effective Density-of-States

Integration over states in energy is a common requirement. To evaluate such integrals analytically for nonparabolic valleys, with DOS given by [Equation 103](#), a first-order Taylor series expansion is applied to the energy terms, resulting in the approximation:

$$\sqrt{\varepsilon(1 + \alpha\varepsilon)}(1 + 2\alpha\varepsilon) = \sqrt{\varepsilon}\left(1 + \frac{5}{2}\alpha\varepsilon\right) \quad (107)$$

Given this approximation, the effective DOS  $N_b$  for a band modeled as a collection of analytic valleys can be defined as:

$$N_b = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{3/2} \sum_i Z_i m_i^{*3/2} \exp(-\Delta E_i)\left(1 + \frac{15}{4}\alpha_i k_B T\right) \quad (108)$$

where the sum is over all valleys in the band model, and  $\Delta E_i$  is related to the difference between the  $i^{\text{th}}$  valley minima and the band edge as:

$$\Delta E_i = \frac{E_i - E_b}{k_B T} \quad (109)$$

[Equation 108](#) is an approximate expression to first order in the nonparabolicity term  $\alpha$ , recovering the exact expression for parabolic bands ( $\alpha = 0$ ), and relates the carrier density to the local band edge  $E_b$  and the Fermi energy  $E_F$  using the band model as:

$$n = N_b \exp\left(\pm \frac{E_b - E_F}{k_B T}\right) \quad (110)$$

where  $\pm$  applies to negatively and positively charged carriers, respectively. [Equation 110](#) applies only when degenerate carrier statistics can be ignored such that the Boltzmann approximation is valid.

---

## Analytic Conduction Band

This section discusses parameters of the analytic conduction band.

## Conduction Band Edge

Given a conduction band defined as a collection of  $N$  analytic valleys, the conduction band edge  $E_C$  is simply defined as the lowest-lying energy minima:

$$E_C = \min\{E_{\min,1}, E_{\min,2}, \dots, E_{\min,N}\} \quad (111)$$

In general, the conduction band edge so defined is not equivalent to the nominal conduction band edge,  $E_{C0}$ , being only equivalent if the energy offset  $\Delta E$  of the lowest valley is zero (see [Figure 35 on page 272](#)).

## Chapter 8: Semiconductor Material Models

### Analytic Valley Model

## Conduction Band Effective Density-of-States

The conduction band effective DOS  $N_C$  for a band modeled as a collection of analytic valleys is given directly from [Equation 108](#) as:

$$N_C = 2 \left( \frac{k_B T}{2\pi\hbar^2} \right)^{3/2} \sum_i Z_i m_i^{3/2} \exp(-\Delta E_i) \left( 1 + \frac{15}{4} \alpha_i k_B T \right) \quad (112)$$

---

## Valence Band

You can model the valence band using either an analytic EMA multivalley model or a six-band  $k \cdot p$  band structure. Consistency between the DOS from the EMA valley and the  $k \cdot p$  band structure is achieved through defining effective masses within the EMA valley model consistently with those determined by the  $k \cdot p$  calculation.

Because of the simplified nature of the EMA valley model, these masses are taken as spherical averages of the  $k \cdot p$  band structure at thermal energy. Carrier dynamics in Monte Carlo simulations can be determined using either the EMA valley model or  $k \cdot p$  model.

---

## Analytic Valence Band

The analytic multivalley model of the valence band follows identically that of the conduction band model and is required to efficiently define the DOS within the valence band for drift-diffusion simulations. [Figure 35 on page 272](#) illustrates the valence band model. The model describes a collection of analytic valleys that approximate the local minima most relevant to carriers within the valence band and defines the DOS in the valence band for drift-diffusion simulations.

## Valence Band Edge

Given a valence band defined as a collection of  $N$  analytic valleys, the valence band edge  $E_V$  is simply defined as the lowest-lying energy minima:

$$E_V = \min\{E_{\min,1}, E_{\min,2}, \dots, E_{\min,N}\} \quad (113)$$

In general, the valence band edge so defined is not equivalent to the nominal valence band edge,  $E_{V0}$ , being only equivalent if the energy offset  $\Delta E$  of the lowest valley is zero (see [Figure 35](#)).

## Chapter 8: Semiconductor Material Models

### Six-Band $k \cdot p$ Band Structure Model

## Valence Band Effective Density-of-States

The valence band effective DOS  $N_V$  for a band modeled as a collection of analytic valleys is given directly from [Equation 108](#) as:

$$N_V = 2 \left( \frac{k_B T}{2\pi\hbar^2} \right)^{3/2} \sum_i Z_i m_i^{*3/2} \exp(-\Delta E_i) \left( 1 + \frac{15}{4} \alpha_i k_B T \right) \quad (114)$$

The DOS effective mass for the  $i^{\text{th}}$  valley  $m_i^*$  can be determined from  $k \cdot p$  band structure models to ensure an equivalent DOS between Monte Carlo and drift-diffusion band models for consistency.

## Six-Band $k \cdot p$ Band Structure Model

A six-band  $k \cdot p$  band structure model allows for the inclusion of spin-orbit coupling and leads to three numeric valence band solutions throughout the Brillouin zone, referred to as the heavy hole (HH) band, the light hole (LH) band, and the spin split off (SSO) band. Such a model accurately represents hole transport that is unobtainable with an analytic multivalley model due to the complicated anisotropic warped nature of valence bands.

Analogously to the analytic multivalley valence band model, the HH, LH, and SSO bands each have an associated energy minima (see [Figure 35 on page 272](#)). In addition, the HH, LH, and SSO bands are linked by a spherically averaged effective mass to a representative valley within the analytic multivalley model. This defines the DOS effective masses for the analytic multivalley model that approximates the DOS from the  $k \cdot p$  band structure.

*Table 36 Parameters of valence band  $k \cdot p$  model*

Parameter symbol	Parameter name	Description	Unit
$L$	<code>L_kp</code>	Sets the $L$ parameter of the model.	$\hbar^2/2m_0$
$M$	<code>M_kp</code>	Sets the $M$ parameter of the model.	$\hbar^2/2m_0$
$N$	<code>N_kp</code>	Sets the $N$ parameter of the model.	$\hbar^2/2m_0$
$l$	<code>L-defpot</code>	Sets the strain deformation potential used to determine the effect of the application of strain.	eV
$m$	<code>M-defpot</code>	Sets the strain deformation potential used to determine the effect of the application of strain.	eV

## Chapter 8: Semiconductor Material Models

### Six-Band $k \cdot p$ Band Structure Model

Table 36 Parameters of valence band  $k \cdot p$  model (Continued)

Parameter symbol	Parameter name	Description	Unit
$n$	N-defpot	Sets the strain deformation potential used to determine the effect of the application of strain.	eV
$\Delta_{\text{so}}$	dss0	Sets the spin split-off energy separation.	eV

## Six-Band $k \cdot p$ Model Parameters

Several parameters define the six-band  $k \cdot p$  band structure (see [Table 32 on page 283](#)). These parameters specify the interaction Hamiltonians for the band-structure model.

For band  $n$ , the dispersion relation  $E_{n,k}$  can be defined following:

$$H u_{n,k} = E_{n,k} u_{n,k} \quad (115)$$

where  $u_{n,k}$  is a function with the same periodicity as the crystal. The Hamiltonian comprising the unstrained Hamiltonian  $H^{k \cdot p}$  and the spin-orbit interactions  $H^{\text{SO}}$  is stated as:

$$H = H^{k \cdot p} + H^{\text{SO}} \quad (116)$$

The unstrained Hamiltonian  $H^{k \cdot p}$  is given as [7]:

$$H^{k \cdot p} = \begin{bmatrix} H & 0 \\ 0 & H \end{bmatrix} \quad (117)$$

where  $H'$  is defined as:

$$H' = \begin{bmatrix} Lk_x^2 + M(k_y^2 + k_z^2) & Nk_xk_y & Nk_xk_z \\ Nk_xk_y & Lk_y^2 + M(k_x^2 + k_z^2) & Nk_yk_z \\ Nk_xk_z & Nk_yk_z & Lk_z^2 + M(k_x^2 + k_y^2) \end{bmatrix} \quad (118)$$

Here,  $L$ ,  $M$ , and  $N$  are the valence band  $k \cdot p$  band-structure parameters.

## Chapter 8: Semiconductor Material Models

### Six-Band $k \cdot p$ Band Structure Model

The spin-orbit perturbation is of the form:

$$H^{\text{so}} = \frac{\Delta_{\text{so}}}{3} \begin{bmatrix} 0 & -i & 0 & 0 & 0 & 1 \\ i & 0 & 0 & 0 & 0 & -i \\ 0 & 0 & 0 & -1 & i & 0 \\ 0 & 0 & -1 & 0 & i & 0 \\ 0 & 0 & -i & -i & 0 & 0 \\ 1 & i & 0 & 0 & 0 & 0 \end{bmatrix} \quad (119)$$

where  $\Delta_{\text{so}}$  is the spin-orbit splitting energy parameter. Following the approach of [8], the exact analytic eigenvalues are precalculated and stored in a spherical polar mesh. In addition, the first derivative of the band structure is stored in order to recover velocities.

## Strain

Strain can be applied within the  $k \cdot p$  band structure by considering the contribution of the strain Hamiltonian  $H^{\text{str}}$  such that the complete interaction Hamiltonian can be stated as:

$$H = H^{k \cdot p} + H^{\text{so}} + H^{\text{str}} \quad (120)$$

The strain contribution is described as:

$$H^{\text{str}} = \begin{bmatrix} H'' & 0 \\ 0 & H'' \end{bmatrix} \quad (121)$$

where  $H''$  is stated as:

$$H'' = \begin{bmatrix} l\varepsilon_{xx} + m(\varepsilon_{yy} + \varepsilon_{zz}) & n\varepsilon_{xy} & n\varepsilon_{xz} \\ n\varepsilon_{xy} & l\varepsilon_{yy} + m(\varepsilon_{xx} + \varepsilon_{zz}) & n\varepsilon_{yz} \\ n\varepsilon_{xz} & n\varepsilon_{yz} & l\varepsilon_{zz} + m(\varepsilon_{xx} + \varepsilon_{yy}) \end{bmatrix} \quad (122)$$

Here,  $l$ ,  $m$ , and  $n$  are the valence band deformation potentials, and  $\varepsilon_{ij}$  is the strain tensor. These additional terms shift the bands, breaking the degeneracy between the HH band and the LH band, and introduces additional band warping that alters the conductivity effective mass and DOS.

## Effective Valence Band Density-of-States

You can define the effective valence band DOS  $N_V$  analogously to the effective conduction band DOS, where summation is performed over all valleys within the valence band model and the reference energy being the valence band edge  $E_V$ :

$$N_V = 2 \left( \frac{k_B T}{2\pi\hbar^2} \right)^{3/2} \sum_i Z_i m_i^{*3/2} \exp(-\Delta E_i) \quad (123)$$

## Chapter 8: Semiconductor Material Models

### Six-Band $k \cdot p$ Band Structure Model

where  $m_i^*$  is the spherically averaged DOS effective mass, defined such that:

$$2\pi\sqrt{E}\left(\frac{m^*}{2\pi^2\hbar^2}\right)^{3/2} = \frac{1}{(2\pi)^3} \int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta k^2 \left|\frac{\partial E}{\partial k}\right|^{-1} \quad (124)$$

Here,  $E$  is the thermal energy, and  $\Delta E_i$  is related to the difference between the  $i^{\text{th}}$  valley minima and the valence band edge as:

$$\Delta E_i = \frac{E_i - E_v}{k_B T} \quad (125)$$

---

## Band Gap

Given the conduction band and valence band models, the band gap  $E_g$  is defined as the difference in energy between the conduction band and valence band edges, as illustrated in [Figure 35 on page 272](#):

$$E_g = E_C - E_V \quad (126)$$

In general, this differs from the nominal band gap  $E_{g0}$  as application of valley offsets, either directly by user-specified alteration or indirectly by application of strain, affects the distribution of the minima within the band models.

---

## Electron Affinity

The electron affinity is determined from the actual conduction band edge  $E_C$ . In general, this differs from the nominal electron affinity  $\chi_0$ , which defines the nominal conduction band edge  $E_{g0}$  as application of valley offsets, either directly by user-specified alteration or indirectly by application of strain, affects the distribution of the minima within the conduction band model.

---

## Intrinsic Carrier Concentration

From the calculation of the effective conduction band and valence band DOS  $N_C$  and  $N_V$ , and given the band gap, the intrinsic carrier concentration  $n_i$  is defined as:

$$n_i = \sqrt{N_C N_V} \exp\left(\frac{1}{2}E_g k_B T\right) \quad (127)$$

which, together with the local electrostatic potential  $V$  and the electron and hole quasi-Fermi levels  $\phi_n$  and  $\phi_p$ , determines the local electron and hole concentrations following the Boltzmann approximation as:

$$n = n_i \exp\left(-\frac{q(V - \phi_n)}{k_B T}\right) \quad (128)$$

## Chapter 8: Semiconductor Material Models

### Interpolation Methods

$$p = n_i \exp\left(-\frac{q(\phi_p - V)}{k_B T}\right) \quad (129)$$

---

## Interpolation Methods

This section describes the interpolation methods used to define some material parameters. These are used, in particular, for binary materials to define parameters based on the constituent materials and a given mole fraction.

---

### Bounded Interpolation

An interpolation method can be bounded so that it applies to a specified range. To specify the bounds, use the following syntax:

```
<parameter> <quantity> <lower_bound> <upper_bound> <scheme> <value>
```

Here, *<quantity>* is the independent variable (for example, mole fraction), and *<scheme>* is the applied interpolation method.

The following example defines the valence band edge of SiGe for mole fractions between 0.2 and 0.6 to use linear interpolation:

```
material SiliconGermanium.valence.E xMoleFraction 0.2 0.6 linear 1.2 -3.1
```

Note the following when defining bounded interpolation:

- If no bounds are defined, then the interpolation applies to the entire range.
- Definitions in the input file overwrite the default over the supplied range, inclusive of both the lower and upper bounds.
- If multiple definitions are supplied that cover a range, then only the lower bound is included.
- The bounds for user definitions cannot overlap.
- You can use a mixture of interpolation methods for a given parameter as long as the ranges do not overlap.

This definition can also be used for fixed fraction  $\text{Si}_{1-x}\text{Ge}_x$  materials. Alternatively, for a single fixed fraction material, the specified interpolation scheme applies to the mole fraction associated with that material.

## Constant Interpolation

This interpolation method is a special case where no interpolation of parameters is applied and no keyword is required as long as the value is an integer or a real number. Optionally, you can specify the `constant` keyword. A fixed (constant) value is used and must be supplied.

The input file syntax for this interpolation is:

```
< parameter > <value>
```

You can also use the `constant` keyword as follows:

```
<parameter> constant <value>
```

The following commands change the effective masses of the G-valley in  $\text{In}_{50}\text{Ga}_{50}\text{As}$  to a constant value:

```
material In50Ga50As.conduction.C1.G.mx 0.043
material In50Ga50As.conduction.C1.G.my 0.043
material In50Ga50As.conduction.C1.G.mz 0.043
```

---

## Linear Interpolation

This interpolation is the default case where a simple linear interpolation of the parameter endpoints is applied. You can either use the parameters from the two constituent pure materials or supply your own endpoints.

The input file syntax to use the constituent material parameters is:

```
<parameter> linear
```

The input file syntax to specify different endpoints is:

```
<parameter> linear <value_A> <value_B>
```

The formula used in linear interpolation is:

$$(1 - x)A + xB \quad (130)$$

The following commands change the effective masses of the G-valley in  $\text{In}_{50}\text{Ga}_{50}\text{As}$  to a linear interpolated value using user-specified endpoints:

```
material In50Ga50As.conduction.C1.G.mx linear 0.03 0.055
material In50Ga50As.conduction.C1.G.my linear 0.03 0.055
material In50Ga50As.conduction.C1.G.mz linear 0.03 0.055
```

## Linear II Interpolation

This interpolation is a rearrangement of linear interpolation. In this case, the two endpoints must be supplied. The input file syntax for this interpolation is:

```
<parameter> linearII <value_A> <value_B>
```

The formula used in this interpolation is:

$$A + xB \quad (131)$$

The following commands change the effective masses of the G-valley in  $\text{In}_{50}\text{Ga}_{50}\text{As}$ :

```
material In50Ga50As.conduction.C1.G.mx linearII 0.03 0.055
material In50Ga50As.conduction.C1.G.my linearII 0.03 0.055
material In50Ga50As.conduction.C1.G.mz linearII 0.03 0.055
```

---

## Piecewise Interpolation

This interpolation can be defined using the following syntax:

```
<parameter> <quantity> <xi> piecewise <value_Pi> <value_Bi> <value_Ci>
```

The value of the independent variable  $x_i$  is required along with  $P_i$ . However, both  $B_i$  and  $C_i$  are optional and define the interpolation between  $x_{i-1}$  and  $x_i$ . Typically, multiple piecewise definitions are given for a parameter to cover a range, and the default interpolation is used outside of any defined range.

The formula for the piecewise form is:

$$\begin{aligned} P &= P_{i-1} + A \cdot \Delta x + B_i \cdot \Delta x^2 + C_i \cdot \Delta x^3 \\ A &= \frac{\Delta P_i}{\Delta x_i} - B_i \cdot \Delta x_i - C_i \cdot \Delta x_i^2 \\ \Delta P_i &= P_i - P_{i-1} \\ \Delta x_i &= x_i - x_{i-1} \\ \Delta x &= x - x_{i-1} \end{aligned} \quad (132)$$

The following commands modify the spin split-off energy between 0.0 and 0.3:

```
material SiliconGermanium.valence.dSSO xMoleFraction 0.0 piecewise 0.0440
material SiliconGermanium.valence.dSSO xMoleFraction 0.1 piecewise 0.0692
material SiliconGermanium.valence.dSSO xMoleFraction 0.2 piecewise 0.0944
material SiliconGermanium.valence.dSSO xMoleFraction 0.3 piecewise 0.1196
```

## Piecewise2 Interpolation

This interpolation is like the piecewise interpolation previously described, but it acts on the squared values of  $P_i$ .

To define this interpolation, use the following syntax:

```
<parameter> <quantity> <xi> piecewise2 <value_Pi> <value_Bi> <value_Ci>
```

For example, to modify the acoustic phonon deformation potential, specify:

```
material SiliconGermanium.valence.HH.vhh.achhlsi.D xMoleFraction 0.0
piecewise2 7.1
material SiliconGermanium.valence.HH.vhh.achhlsi.D xMoleFraction 1.0
piecewise2 0.0
```

---

## Fixed Linear Interpolation

This interpolation method is a special case where a fixed interpolation point for the linear interpolation is used. The following use cases apply to this interpolation method:

- Using pure material parameters as the endpoints
- Specifying the endpoints

The input file syntax using constituent material endpoints is:

```
<parameter> fixed <x_fraction>
```

The input file syntax for user-defined value endpoints is:

```
<parameter> fixed <x_fraction> <value_A> <value_B>
```

The linear interpolation formula of [Equation 130 on page 302](#) is used.

The following commands change the effective masses of the X1 valley in In<sub>50</sub>Ga<sub>50</sub>As to a fixed linear interpolation value of  $x = 0$ :

```
material In50Ga50As.conduction.C1.X1.mx fixed 0.0      # Use InAs mass
material In50Ga50As.conduction.C1.X1.my fixed 0.0      # Use InAs mass
material In50Ga50As.conduction.C1.X1.mz fixed 0.0      # Use InAs mass
```

The following commands change the effective masses of the X1 valley in In<sub>50</sub>Ga<sub>50</sub>As to a fixed linear interpolation value of  $x = 0.2$  with user-defined endpoints:

```
material In50Ga50As.conduction.C1.X1.mx fixed 0.2 1.60 2.02
material In50Ga50As.conduction.C1.X1.my fixed 0.2 0.22 0.35
material In50Ga50As.conduction.C1.X1.mz fixed 0.2 0.22 0.35
```

## Quadratic I Interpolation

This interpolation method uses a quadratic formula that includes a bowing parameter.

The following use cases apply to this interpolation method:

- Only the bowing parameter is supplied and the constituent material parameters are used as endpoints.
- The endpoints and the bowing parameter are specified.

The input file syntax to use when only the bowing parameter is supplied is:

```
<parameter> quadraticI <C>
```

The input file syntax to use when specifying user-defined value endpoints is:

```
<parameter_name> quadraticI <value_A> <value_B> <C>
```

The formula for this interpolation method is:

$$(1 - x)A + xB + x(1 - x)C \quad (133)$$

The following command changes the valley energy of the valence SSO valley in In<sub>50</sub>Ga<sub>50</sub>As to a quadratic interpolation with a bowing value of C = -0.15 :

```
material In50Ga50As.valence.SSO.E quadraticI -0.15 # Energy from min
```

The following command changes the valley energy of the valence SSO valley in In<sub>50</sub>Ga<sub>50</sub>As to a quadratic interpolation with user-defined endpoints for interpolation:

```
material In50Ga50As.valence.SSO.E quadraticI 0.35 0.62 -0.15
```

---

## Quadratic II Interpolation

This interpolation method uses a quadratic formula for interpolation that is essentially a rearrangement of the quadratic I formula.

The following use cases apply to this interpolation method:

- Only the bowing parameter is supplied and the constituent material parameters are used as endpoints.
- The endpoints and the bowing parameter are specified.

The input file syntax to use when only the bowing parameter is supplied is:

```
<parameter> quadraticII <C>
```

The input file syntax to use when specifying user-defined value endpoints is:

```
<parameter> quadraticII <value_A> <value_B> <C>
```

## Chapter 8: Semiconductor Material Models

### References

The formula for this interpolation method is:

$$A + (B - A)x^2 + x(1 - x)C \quad (134)$$

The following command changes the valley energy of the valence SSO valley in In<sub>50</sub>Ga<sub>50</sub>As to a quadratic interpolation with a bowing value of  $C = -0.15$ :

```
material In50Ga50As.valence.SSO.E quadraticII -0.15
```

The following command changes the valley energy of the valence SSO valley in In<sub>50</sub>Ga<sub>50</sub>As to a quadratic interpolation with user-defined endpoints for interpolation:

```
material In50Ga50As.valence.SSO.E quadraticII 0.35 0.62 -0.15
```

---

## Quadratic III Interpolation

This interpolation method uses a quadratic formula that is essentially a rearrangement of the quadratic I formula. In this case, two endpoints and the bowing parameter must be supplied.

The input file syntax for this interpolation method is:

```
<parameter> quadraticIII <value_A> <value_B> <C>
```

The formula for this interpolation method is:

$$A + Bx + Cx^2 \quad (135)$$

The following command changes the valley energy of the valence SSO valley in In<sub>50</sub>Ga<sub>50</sub>As to a quadratic interpolation with a bowing value of  $C = -0.15$ :

```
material In50Ga50As.valence.SSO.E quadraticIII 0.35 0.62 -0.15
```

---

## References

- [1] C. Jacoboni and P. Lugli, *The Monte Carlo Method for Semiconductor Device Simulation*, Computational Microelectronics, Wien: Springer, 1989.
- [2] M. L. Lee *et al.*, “Strained Si, SiGe, and Ge channels for high-mobility metal-oxide-semiconductor field-effect transistors,” *Journal of Applied Physics*, vol. 97, no. 1, p. 011101, 2005.
- [3] S. Smirnov, H. Kosina, and S. Selberherr, “Substrate Orientation-Dependence of Electron Mobility in Strained SiGe Layers,” in *International Conference on Simulation of Semiconductor Processes and Devices (SISPAD)*, Boston, MA, USA, pp. 55–58, September 2003.
- [4] D. Rideau *et al.*, “Strained Si, Ge, and Si<sub>1-x</sub>Ge<sub>x</sub> alloys modeled with a first-principles-optimized full-zone  $k\cdot p$  method,” *Physical Review B*, vol. 74, no. 19, p. 195208, 2006.

## Chapter 8: Semiconductor Material Models

### References

- [5] V. Sverdlov, "Strain and Stress," *Strain-Induced Effects in Advanced MOSFETs*, Computational Microelectronics, Wien: Springer, pp. 23–34, 2011.
- [6] E. Ungersboeck *et al.*, "The Effect of General Strain on the Band Structure and Electron Mobility of Silicon," *IEEE Transactions on Electron Devices*, vol. 54, no. 9, pp. 2183–2190, 2007.
- [7] J. M. Hinckley and J. Singh, "Hole transport theory in pseudomorphic  $\text{Si}_{1-x}\text{Ge}_x$  alloys grown on Si(001) substrates," *Physical Review B*, vol. 41, no. 5, pp. 2912–2926, 1990.
- [8] J. E. Dijkstra and W. Th. Wenckebach, "Hole transport in strained Si," *Journal of Applied Physics*, vol. 81, no. 3, pp. 1259–1263, 1997.

# 9

## Insulator Material Models

---

This chapter describes the general insulator material models that Garand uses.

---

### Definition of Insulator Material Models

Garand provides default models for common insulator materials (see [Default Insulator Materials on page 382](#)). An insulator material model defines a set of parameters, with each default insulator material having its own set of default parameter values.

The insulator material model definition consists fundamentally of the following separate models:

- The *bulk material model* defines a set of bulk material values.
- The *band structure model* defines a nominal band-edge model with respect to vacuum to define band discontinuities.

---

### Bulk Material Model

This model consists of a list of bulk material parameters that describe the electrical properties of the insulator.

Table 37     *Parameter of bulk material model*

Parameter symbol	Parameter name	Description	Unit
$\kappa$	permittivity	Sets the scalar static relative dielectric constant.	–

See [Default Insulator Materials on page 382](#) for the default bulk material parameter values for each insulator material model.

## Changing Default Parameter Values

To change the default parameter values of the bulk material in the input file, use the following syntax:

```
material <material>.<parameter> <value>
```

where:

- **<material>** is the name of a material listed in [Table 66 on page 382](#).
- **<parameter>** is the name of a parameter listed in [Table 37 on page 308](#).
- **<value>** is the new value of the parameter, specified with the expected type and format.

### Example

Define the permittivity of Oxide to be 2.0:

```
material Oxide.permittivity 2.0
```

---

## Band Structure Model

This section describes the band structure model.

---

### Band Container Model

[Table 38](#) lists the parameters of the nominal band edge model, which are conduction band and valence band edge properties.

*Table 38 Parameters of nominal band edge model*

Parameter symbol	Parameter name	Description	Unit
$E$	E	Sets the energy of the band edge relative to the vacuum level.	eV
$m_{dg_x}$	dgx	Sets the x-component of the density-gradient effective mass for carriers associated with the band.	$m_e$
$m_{dg_y}$	dgy	Sets the y-component of the density-gradient effective mass for carriers associated with the band.	$m_e$
$m_{dg_z}$	dgz	Sets the z-component of the density-gradient effective mass for carriers associated with the band.	$m_e$

## Chapter 9: Insulator Material Models

### Band Structure Model

See [Default Insulator Materials on page 382](#) for the default material band-edge parameter values for each insulator material model.

## Changing Default Parameter Values

To change the default parameter values in the input file, use the following syntax:

```
material <material>.<bandcontainer>.<parameter> <value>
```

where:

- <material> is the name of a material listed in [Table 66 on page 382](#).
- <bandcontainer> is either conduction or valence.
- <parameter> is the name of a parameter listed in [Table 38](#).
- <value> is the new value of the parameter, specified with the expected type and format.

### Example

Define the conduction band edge of Oxide to be 5.0 eV below the vacuum level and the x-component of the density-gradient effective mass in the valence band to be 0.47  $m_e$ :

```
material Oxide.conduction.E 5.00
material Oxide.valence.dgx 0.47
```

---

## Nominal Valley Model

The nominal valley model defines the effective masses for insulator materials that are used in Schrödinger solutions.

*Table 39 Parameters of nominal valley model*

Parameter symbol	Parameter name	Description	Unit
$m_x$	mx	Sets the <i>longitudinal</i> effective mass (aligning the longitudinal axis with the Cartesian x-axis).	$m_e$
$m_y$	my	Sets the <i>transverse</i> effective mass (aligning the transverse axis with the Cartesian y-axis).	$m_e$
$m_z$	mz	Sets the <i>transverse</i> effective mass (aligning the transverse axis with the Cartesian z-axis).	$m_e$

## Chapter 9: Insulator Material Models

### Band Structure Model

Table 39 Parameters of nominal valley model (Continued)

Parameter symbol	Parameter name	Description	Unit
$m_{qx}$	<code>mqx</code>	Sets the confinement effective mass along the x-axis of the device. This is set automatically based on the crystal orientation, but it can be changed to suit the user specification.	$m_e$
$m_{qy}$	<code>mqy</code>	Sets the confinement effective mass along the y-axis of the device. This is set automatically based on the crystal orientation, but it can be changed to suit the user specification.	$m_e$
$m_{qz}$	<code>mqz</code>	Sets the confinement effective mass along the z-axis of the device. This is set automatically based on the crystal orientation, but it can be changed to suit the user specification.	$m_e$

See [Default Insulator Materials on page 382](#) for the default analytic valley parameter values for each insulator material model.

## Changing Default Parameter Values

To change the default parameter values in the input file, use the following syntax:

```
material <material>. <bandcontainer>. <band>. <valley>. <parameter> <value>
```

where:

- `<material>` is the name of a material listed in [Table 66 on page 382](#).
- `<bandcontainer>` is either `conduction` or `valence`.
- `<band>` is the name of a band in the band container.
- `<valley>` is the name of a valley minimum.
- `<parameter>` is the name of a parameter listed in [Table 39](#).
- `<value>` is the new value of the parameter, specified with the expected type and format.

## **Chapter 9: Insulator Material Models**

### Band Structure Model

#### **Example**

Define the effective masses in the x-, y-, z-axes of the valley as 0.85, 0.45, and  $0.30 m_e$ , respectively:

```
material Oxide.conduction.C1.C.mx 0.85
material Oxide.conduction.C1.C.my 0.45
material Oxide.conduction.C1.C.mz 0.30
```

# 10

## Mobility Models

---

*This chapter describes the mobility models that define carrier transport in drift-diffusion simulations. The discussion of these models and their applications applies equally to carrier transport in conduction bands and valence bands, although default parameter values of mobility models differ in each case.*

---

### Semiconductor Material Mobility Models

Each band within a semiconductor material model defines a mobility model. The mobility model is defined by the combination of three models, each of which defines mobility with respect to one of the following transport regimes:

- Low-field mobility
- Perpendicular field–dependent mobility
- Lateral field–dependent mobility

Evaluation of low-field mobility results in a value that becomes an argument to the perpendicular field–dependent mobility model, the result of which then becomes an argument to the lateral field–dependent mobility model. In this way, the final mobility depends on the specific models selected in all three regimes.

In addition to these models, you can specify a ballistic mobility model that is applied using Matthiessen’s rule after all other models.

Multiple models can be applied to each regime, but only one model can be selected as part of the complete mobility model.

---

### Specifying Nondefault Mobility Models

#### Note:

See Part IV for the default mobility models for different semiconductor material models.

## Chapter 10: Mobility Models

### Semiconductor Material Mobility Models

To specify nondefault material mobility models in the input file, use the following syntax:

```
material <material>.⟨bandcontainer⟩.mobility.⟨model⟩ <value>
```

where:

- <material> is the name of a material (see [Semiconductor Materials on page 842](#)).
- <bandcontainer> is either conduction or valence.
- <model> is the name of a model listed in [Table 40](#).
- <value> must be the name of a previously defined mobility model appropriate to the model type or NONE.

*Table 40 Parameters for specifying the type of mobility model*

Model type	Model name	Description
Bulk	bulk	Name of a bulk low-field mobility model
Perpendicular field	eprp	Name of a perpendicular field-dependent mobility model
Lateral field	elat	Name of a lateral field-dependent mobility model
Ballistic	ball	Name of a ballistic mobility model
Strain	strain	Name of a strain-dependent mobility model

#### Example

```
material Silicon.conduction.mobility.bulk      Masetti
material Silicon.conduction.mobility.eprp       NONE
material Silicon.conduction.mobility.elat       Caughey
material Silicon.conduction.mobility.ball       NONE
material Silicon.conduction.mobility.strain    Multivalley
```

These commands define that the mobility model for carriers within the silicon conduction band will use the Masetti model for low-field concentration-dependent mobility, with no dependence on the perpendicular field, and will use the Caughey–Thomas mobility model for the lateral field dependence, and no ballistic mobility model.

---

## Low-Field Mobility Models

Low-field mobility defines the base mobility that is subsequently modified by the perpendicular field-dependent mobility model. The following models are available:

- [Constant Mobility Model](#)
- [Arora Mobility Model](#)
- [Masetti Mobility Model](#)
- [Philips Unified Mobility Model](#)

---

### Constant Mobility Model

Constant mobility defines an isotropic low-field mobility value  $\mu_c$  that is applied globally throughout the simulation domain:

$$\mu_0 = \mu_c \quad (136)$$

*Table 41 Parameter of constant mobility model as defined in [Equation 136](#)*

Parameter symbol	Parameter name	Description	Type	Unit
$\mu_0$	mu0	Constant low-field mobility	float	$\text{cm}^2/\text{Vs}$
$\zeta$	zeta	Fitting parameter	float	—

### Changing Default Parameter Values

**Note:**

See Part IV for the default parameter values for different semiconductor material models.

To change the default parameter values for this mobility model in the input file, use the following syntax:

```
material <material>. <bandcontainer>.constant.<parameter> <value>
```

**Example**

Set the constant mobility for electrons as  $1500 \text{ cm}^2/\text{Vs}$  and for holes as  $300 \text{ cm}^2/\text{Vs}$  in silicon:

```
material Silicon.conduction.constant.mu0 1500  
material Silicon.valence.constant.mu0 300
```

## Chapter 10: Mobility Models

### Low-Field Mobility Models

#### Arora Mobility Model

Similar to the Masetti model, the Arora concentration-dependent mobility model [1] defines a local mobility, dependent on the local total doping density  $N_{\text{tot}}$ , by an analytic fit to electron and hole mobilities in doped silicon over a wide range of doping densities and temperatures. It is given as:

$$\mu_0 = \mu_{\min} T'_1 + \frac{(\mu_{\max} - \mu_{\min}) T'_2}{1 + \left( \frac{N_{\text{tot}}}{N_0 T'_3} \right)^{\alpha}} \quad (137)$$

where  $\alpha = AT'_4$  and  $T'_i = \left( \frac{T}{300} \right)^{\beta_i}$ .

Table 42 Parameters of Arora mobility model as defined in Equation 137

Parameter symbol	Parameter name	Description	Type	Unit
$\mu_{\min}$	mumin	Minimum mobility	float	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	float	$\text{cm}^2/\text{Vs}$
$N_0$	n0	Reference concentration	float	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	float	—
$\beta_1$	b1	Fitting parameter	float	—
$\beta_2$	b2	Fitting parameter	float	—
$\beta_3$	b3	Fitting parameter	float	—
$\beta_4$	b4	Fitting parameter	float	—

#### Changing Default Parameter Values

##### Note:

See Part IV for the default parameter values for different semiconductor material models.

## Chapter 10: Mobility Models

### Low-Field Mobility Models

To change the default parameter values for this mobility model in the input file, use the following syntax:

```
material <material>.<bandcontainer>.Arora.<parameter> <value>
```

#### Example

Set the values of  $\mu_{\max}$  to  $800 \text{ cm}^2/\text{Vs}$ ,  $N_0$  to  $5.0 \times 10^{16} \text{ cm}^{-3}$ , and  $\beta_1$  to  $-0.4$ , for electrons in silicon:

```
material Silicon.conduction.arora.mumax 800
material Silicon.conduction.arora.n0      5.0e16
material Silicon.conduction.arora.b1     -0.4
```

---

## Masetti Mobility Model

The Masetti concentration-dependent mobility model [2] defines electron and hole mobility by using an analytic function that fits empirical electron mobilities in bulk arsenic-doped and phosphorus-doped silicon, and hole mobilities in bulk boron-doped silicon over a wide range of doping densities.

They are given as follows for electron and hole mobilities, respectively:

$$\mu_n = \mu_{\min} + \frac{\mu_{\max} - \mu_{\min}}{1 + \left(\frac{n}{C_r}\right)^\alpha} - \frac{\mu_1}{1 + \left(\frac{C_s}{n}\right)^\beta} \quad (138)$$

$$\mu_p = \mu_{\min} e^{-\frac{p_c}{N_D}} + \frac{\mu_{\max}}{1 + \left(\frac{p}{C_r}\right)^\alpha} - \frac{\mu_1}{1 + \left(\frac{C_s}{p}\right)^\beta} \quad (139)$$

where  $n$  and  $p$  are the electron and hole carrier densities.

These functions are implemented as a single function for both electrons and holes, dependent on the local total doping density  $N_{\text{tot}}$  within the simulation domain, and incorporating the power law temperature dependence of the phonon-limited maximum mobility  $\mu_{\max}$  as proposed in [3]:

$$\mu_0 = \mu_{\min1} e^{-\frac{p_c}{N_{\text{tot}}} + \frac{\mu_{\max} \left(\frac{T}{300}\right)^{-\zeta} - \mu_{\min2}}{1 + \left(\frac{N_{\text{tot}}}{C_r}\right)^\alpha}} - \frac{\mu_1}{1 + \left(\frac{C_s}{N_{\text{tot}}}\right)^\beta} \quad (140)$$

When  $\mu_{\min1} = \mu_{\min2}$  and  $p_c = 0$ , Equation 138 is recovered. When  $p_c > 0$  and  $\mu_{\min2} = 0$ , Equation 139 is recovered.

## Chapter 10: Mobility Models

### Low-Field Mobility Models

Table 43 Parameters of Masetti mobility model as defined in [Equation 140](#)

Parameter symbol	Parameter name	Description	Type	Unit
$\mu_{\min 1}$	mumin1	Minimum mobility	float	cm <sup>2</sup> /Vs
$\mu_{\min 2}$	mumin2	Minimum mobility	float	cm <sup>2</sup> /Vs
$\mu_{\max}$	mumax	Maximum mobility	float	cm <sup>2</sup> /Vs
$\mu_1$	mul	Maximum mobility	float	cm <sup>2</sup> /Vs
$C_r$	cr	Reference concentration	float	cm <sup>-3</sup>
$C_s$	cs	Reference solid solubility concentration	float	cm <sup>-3</sup>
$p_c$	pc	Reference concentration	float	cm <sup>-3</sup>
$\alpha$	alpha	Fitting parameter	float	—
$\beta$	beta	Fitting parameter	float	—
$\zeta$	zeta	Fitting parameter	float	—

## Changing Default Parameter Values

### Note:

See Part IV for the default parameter values for different semiconductor material models.

To change the default parameter values for this mobility model in the input file, use the following syntax:

```
material <material>.<bandcontainer>.Masetti.<parameter> <value>
```

### Example

Set the values of  $\mu_{\max}$  to 800 cm<sup>2</sup>/Vs,  $\mu_{\min 1}$  to 400 cm<sup>2</sup>/Vs, and  $\alpha$  to 0.2, for electrons in silicon:

```
material Silicon.conduction.masetti.mumax 800
material Silicon.conduction.masetti.mumin1 400
material Silicon.conduction.masetti.alpha 0.2
```

## Chapter 10: Mobility Models

### Low-Field Mobility Models

## Philips Unified Mobility Model

The Philips unified mobility model [4] is concentration dependent and defines the low-field carrier mobility using an analytic function that takes into account the following:

- Scattering by acceptors (A) and donors (D)
- Carrier-carrier scattering and screening

The electron mobility is expressed as:

$$\frac{1}{\mu_n} = \frac{1}{\mu_{n, \text{lattice}}} + \frac{1}{\mu_{A+D+p}} \quad (141)$$

where:

$$\mu_{n, \text{lattice}} = \mu_{\max} \left( \frac{T}{300} \right)^{-2.285} \quad (142)$$

$$\mu_{A+D+p} = \mu_{1,n} \left( \frac{N_{sc,n}}{N_{sc,eff,n}} \right) \left( \frac{N_{ref}}{N_{sc,n}} \right)^\alpha + \mu_{2,n} \left( \frac{n+p}{N_{sc,eff,n}} \right) \quad (143)$$

where  $n$  and  $p$  are the electron and hole carrier densities, and  $\mu_{1,n}$  and  $\mu_{2,n}$  are parameters defined as:

$$\mu_{1,n} = \frac{\mu_{\max}^2}{\mu_{\max} - \mu_{\min}} \left( \frac{T}{300} \right)^{3\alpha - 1.5} \quad (144)$$

$$\mu_{2,n} = \frac{\mu_{\max} \mu_{\min}}{\mu_{\max} - \mu_{\min}} \left( \frac{300}{T} \right)^{0.5} \quad (145)$$

$N_{sc,n}$  and  $N_{sc,eff,n}$  represent the concentration and the effective concentration to be used in the impurity-carrier scattering, and they are corrected to take into account ultrahigh doping effects:

$$N_{sc,n} = N_D^* + N_A^* + p \quad (146)$$

$$N_{sc,eff,n} = N_D^* + N_A^* G(P_n) + \frac{p}{F(P_n)} \quad (147)$$

where the ultrahigh doping corrections come through:

$$N_D^* = N_D \left( 1 + \frac{1}{C_D + \left( \frac{N_{D,ref}}{N_D} \right)^2} \right) \quad (148)$$

$$N_A^* = N_A \left( 1 + \frac{1}{C_A + \left( \frac{N_{A,ref}}{N_A} \right)^2} \right) \quad (149)$$

## Chapter 10: Mobility Models

### Low-Field Mobility Models

The analytic functions  $G(P_n)$  and  $F(P_n)$  describe the minority carrier scattering by impurities and the electron–hole scattering, respectively:

$$G(P_n) = 1 - \frac{0.89233}{\left[0.41372 + P_n \left(\frac{m_0}{m_e} \frac{T}{300}\right)^{0.28227}\right]^{0.19778}} + \frac{0.005978}{\left[P_n \left(\frac{m_e}{m_0} \frac{T}{300}\right)^{0.72169}\right]^{1.80618}} \quad (150)$$

$$F(P_n) = \frac{2.2999 + 0.7643 P_n^{0.6478} + 6.5502 \frac{m_e}{m_h}}{2.3670 + P_n^{0.6478} - 0.8552 \frac{m_e}{m_h}} \quad (151)$$

The screening parameter is expressed as the weighted average of the Conwell–Weisskopf screening [5] and the Brooks–Herring screening [5]:

$$P_n = \left[ \frac{f_{CW}}{N_{sc, ref} N_{sc, n}^{-2/3}} + \frac{f_{BH}}{\frac{N_{c, ref} \left(\frac{m_e}{m_0}\right)}{n + p} \left(\frac{T}{300}\right)^2} \right]^{-1} \quad (152)$$

The same expressions hold for holes, with the opportune change of subscript notation.

*Table 44 Parameters of Philips unified mobility model*

Parameter symbol	Parameter name	Description	Type	Unit
$\mu_{min}$	mumin	Minimum mobility	float	$\text{cm}^2/\text{Vs}$
$\mu_{max}$	mumax	Maximum mobility	float	$\text{cm}^2/\text{Vs}$
$\alpha$	alpha	Fitting parameter	float	–
$C_D$	CD	Reference concentration for ultrahigh-doped donors	float	–
$C_A$	CA	Reference concentration for ultrahigh- doped acceptors	float	–
$N_{ref}$	Nref	Reference concentration	float	$\text{cm}^{-3}$
$N_{D, ref}$	NDref	Reference concentration	float	$\text{cm}^{-3}$
$N_{A, ref}$	NAref	Reference concentration	float	$\text{cm}^{-3}$
$N_{c, ref}$	Ncref	Reference concentration	float	$\text{cm}^{-3}$

## Chapter 10: Mobility Models

### Low-Field Mobility Models

Table 44 Parameters of Philips unified mobility model (Continued)

Parameter symbol	Parameter name	Description	Type	Unit
$N_{sc, ref}$	<code>Nscref</code>	Reference surface concentration	float	$\text{cm}^{-2}$
$m_e$	<code>me</code>	Normalized electron mass	float	—
$m_h$	<code>mh</code>	Normalized hole mass	float	—
$f_{BH}$	<code>fbh</code>	Brooks–Herring coefficient	float	—
$f_{CW}$	<code>fcw</code>	Conwell–Weisskopf coefficient	float	—

## Changing Default Parameter Values

### Note:

See Part IV for the default parameter values for different semiconductor material models.

To change the default parameter values for this mobility model in the input file, use the following syntax:

```
material <material>.bandcontainer.Philips.<parameter> <value>
```

### Example

Set the values of  $\mu_{\max}$  to  $800 \text{ cm}^2/\text{Vs}$ ,  $\mu_{\min}$  to  $400 \text{ cm}^2/\text{Vs}$ , and  $\alpha$  to 1.2, for electrons in silicon:

```
material Silicon.conduction.philips.mumax 800
material Silicon.conduction.philips.mumin 400
material Silicon.conduction.philips.alpha 1.2
```

---

## Low-Field Mobility Modifiers

The `strainx` and `rsx` modifiers scale the low-field mobility by a fixed value in different regions of the device. These can be useful as calibration parameters.

## Chapter 10: Mobility Models

### Low-Field Mobility Models

#### The strainx Modifier

This modifier is a scaling factor that multiplies the low-field mobility in the channel region of the MOSFET being simulated. It is intended to be used as a simple mechanism to approximate the effects of strain on the channel mobility.

The channel region is determined to be any region in the device where the majority-type doping is less than the limit set by the parameter `strainx_doping_limit` of the `model` command. The low-field mobility for the doping concentration `strainx_doping_limit` is calculated as the mobility for the doping concentration at a given node. The difference between these two mobilities is then scaled by `strainx`, that is:

$$\mu^*(N) = \mu(\text{strainx\_doping\_limit}) + \text{strainx} \\ \times (\mu(N) - \mu(\text{strainx\_doping\_limit}))$$

where  $N$  is the majority-type doping at the node being considered (that is,  $N_D$  in an NMOS device or  $N_A$  in a PMOS device).

The input file command to set the value of `strainx` for a particular material and carrier type is:

```
material <material>.<bandcontainer>.mobility.strainx <value>
```

The following command uses the value specified to scale the low-field channel mobility of electrons in silicon:

```
material Silicon.conduction.mobility.strainx <value>
```

By default, the value of `strainx_doping_limit` is  $10^{20} \text{ cm}^{-3}$ . You can change this with the command:

```
model strainx_doping_limit=<float>
```

#### The rsx Modifier

This modifier is a scaling factor that multiplies the low-field mobility in the source/drain regions of the MOSFET being simulated. It is intended to be used as a simple mechanism to adjust the access resistance of source/drain regions.

Source/drain regions are determined by whether the majority-type doping at a given point is higher than  $5 \times 10^{19} \text{ cm}^{-3}$ . If so, then `rsx` is applied fully. At lower doping concentrations, the effect of `rsx` is reduced so that it has no effect at doping concentrations below  $10^{17} \text{ cm}^{-3}$ .

To set the value of `rsx` for a particular material and carrier type, use the following input file command:

```
material <material>.<bandcontainer>.mobility.rsx <value>
```

## Chapter 10: Mobility Models

### Perpendicular Field–Dependent Mobility Models

The following command uses the value specified to scale the low-field source/drain mobility of holes in silicon:

```
material Silicon.valence.mobility.rsx <value>
```

---

## Perpendicular Field–Dependent Mobility Models

Applying a perpendicular field–dependent mobility model modifies the low-field mobility to reflect surface scattering effects from semiconductor–insulator interfaces. The resulting perpendicular field–dependent mobility  $\mu_{\perp}$ , in turn, is modified by the selected lateral field–dependent mobility model. The following models are available:

- [No Model](#)
- [Yamaguchi Mobility Model](#)
- [Lombardi Mobility Model](#)
- [Thin-Layer Mobility Model](#)

---

## Calculation of the Perpendicular Electric Field

The electric field used for the perpendicular field–dependent mobility models is based on the gradient of the electrostatic potential. The directional component of this field that is considered to be *perpendicular* can be selected from the following options:

- Normal to the nearest interface
- Normal to the direction of current flow

You specify the option with the following command in the Garand input file:

```
model eprp_method=<string>
```

where `<string>` can be `normal_to_interface` (default) or `normal_to_current`.

---

## No Model

Specifying `NONE` means that no perpendicular dependence of the electric field is accounted for and the low-field mobility remains unmodified, such that:

$$\mu_{\perp} = \mu_0 \tag{153}$$

## Yamaguchi Mobility Model

The Yamaguchi mobility model [6] is an empirical model that fits the degradation of the inversion layer mobility as an increasing function of the confinement field, perpendicular to the motion of carriers. It is expressed as:

$$\mu_{\perp}(E_{\perp}) = \frac{\mu_0}{\sqrt{1 + D^2 \left(\frac{E_{\perp}}{E_c}\right)^{\alpha}}} \quad (154)$$

where:

- $\mu_0$  is the mobility resulting from a previously evaluated low-field mobility model.
- $E_c$  is the critical electric field used as a fitting parameter for the model.
- $\alpha$  is a secondary fitting parameter.
- $D = \exp\left(\frac{-l}{l_{\text{crit}}}\right)$  is an empirical depth dependence that ensures the surface mobility reduction mainly affects carriers close to semiconductor–insulator interfaces.

*Table 45 Parameters of Yamaguchi mobility model as defined in Equation 154*

Parameter symbol	Parameter name	Description	Type	Unit
$E_c$	ec	Critical field	float	V/cm
$\alpha$	alpha	Fitting parameter	float	—

## Changing Default Parameter Values

### Note:

See Part IV for the default parameter values for different semiconductor material models.

To change the default parameter values for this mobility model in the input file, use the following syntax:

```
material <material>.bandcontainer.yamaguchi.<parameter> <value>
```

### Examples

Set the value of  $E_c$  for electrons in silicon to 5900 V/cm:

```
material Silicon.conduction.yamaguchi.ec 5.9e5
```

## Chapter 10: Mobility Models

### Perpendicular Field–Dependent Mobility Models

Set the value of  $\alpha$  for electrons in silicon to 2:

```
material Silicon.conduction.yamaguchi.alpha 2.e0
```

---

## Lombardi Mobility Model

The Lombardi mobility model [3] is a semiempirical model that combines bulk low-field mobility with temperature-dependent surface acoustic phonon-limited mobility and a surface roughness–limited mobility that takes into account the confinement field in a similar way to the Yamaguchi mobility model (see [Yamaguchi Mobility Model on page 324](#)).

The model follows the modifications to the original Lombardi model proposed in [7]. It is expressed as:

$$\mu_{\perp} = \left( \frac{1}{\mu_0} + \frac{D}{\mu_{ac}} + \frac{D}{\mu_{sr}} \right)^{-1} \quad (155)$$

where:

- $\mu_0$  is the mobility resulting from a previously evaluated low-field mobility model.
- $\mu_{ac}$  is the surface acoustic–limited mobility, given by  $\mu_{ac} = \frac{B}{E_{\perp}} + \frac{CN_{tot}^{\lambda}}{T^{\kappa} E_{\perp}^{1/3}}$ .
- $\mu_{sr}$  is the surface roughness–limited mobility, given by  $\mu_{sr} = \left( \frac{E_{\perp}^{\gamma}}{\delta} + \frac{E_{\perp}^3}{\eta} \right)^{-1}$ , where  $\gamma$  is defined as  $\gamma = A + \frac{\alpha n}{N_{tot}^{\nu}}$ .
- $D = \exp\left(\frac{-l}{l_{crit}}\right)$  is an empirical depth dependence that ensures the surface mobility reduction degrades as the carrier separation from the surface increases.

Table 46 Parameters of Lombardi mobility model as defined in [Equation 155](#)

Parameter symbol	Parameter name	Description	Type	Unit
A	a	Fitting parameter	float	—
B	b	Fitting parameter	float	cm/s
C	c	Fitting parameter	float	cm <sup>5/3</sup> V <sup>-2/3</sup> s <sup>-1</sup>

## Chapter 10: Mobility Models

### Perpendicular Field–Dependent Mobility Models

Table 46 Parameters of Lombardi mobility model as defined in [Equation 155](#) (Continued)

Parameter symbol	Parameter name	Description	Type	Unit
$\alpha$	alpha	Fitting parameter	float	$\text{cm}^3$
$\delta$	delta	Fitting parameter	float	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	float	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	float	—
$\lambda$	lambda	Fitting parameter	float	—
$\nu$	nu	Fitting parameter	float	—
$N_0$	n0	Fitting parameter	float	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	float	$\text{cm}^{-3}$
$l_{\text{crit}}$	lcrit	Fitting parameter	float	cm

## Changing Default Parameter Values

### Note:

See Part IV for the default parameter values for different semiconductor material models.

To change the default parameter values for this mobility model in the input file, use the following syntax:

```
material <material>. <bandcontainer>.Lombardi.<parameter> <value>
```

### Example

Set the value of  $\delta$  for electrons in silicon to  $6.0 \times 10^{14} \text{ cm}^2/\text{Vs}$ :

```
material Silicon.conduction.lombardi.delta 6.0e14
```

---

## Thin-Layer Mobility Model

The thin-layer mobility model [8] can be considered an extension of the Lombardi mobility model. It is usually applied to devices featuring a silicon body that is a few nanometers thick.

## Chapter 10: Mobility Models

### Perpendicular Field–Dependent Mobility Models

Because of the quantum effects of the inversion charge distribution, the scattering rate is a function of the silicon thickness. The thin-layer mobility model takes into account the following contributions to scattering:

- Bulk phonon scattering
- Surface roughness scattering
- Thickness fluctuation scattering
- Surface phonon scattering

The model is expressed as:

$$\mu_{\perp} = \left( \frac{1}{\mu_0} + \frac{D}{\mu_{bp}} + \frac{D}{\mu_{sr}} + \frac{D}{\mu_{tf}} + \frac{D}{\mu_{sp}} \right)^{-1} \quad (156)$$

where:

- $\mu_0$  is the mobility resulting from a previously evaluated low-field mobility model.
- $D = \exp\left(\frac{-l}{l_{crit}}\right)$  is an empirical depth dependence that ensures the perpendicular-field mobility reduction degrades as the carrier separation from the surface increases.
- The surface roughness–limited mobility  $\mu_{sr}$  is given by the Lombardi mobility model,

$$\mu_{sr} = \left( \frac{E_{\perp}^{\zeta}}{\delta} + \frac{E_{\perp}^3}{\eta} \right)^{-1}, \text{ where } \zeta \text{ is defined as } \zeta = A + \frac{\alpha n}{N_{tot}^v}.$$

- The thickness fluctuation–limited mobility  $\mu_{tf}$  is given by  $\mu_{tf} = \mu_{tf0} \left( \frac{t_b}{1 \text{ nm}} \right)^6 \left[ 1 + \frac{F_{\perp}}{F_{tf0}} \right]$ .
- The surface phonon–limited mobility  $\mu_{sp}$  is given by  $\mu_{sp} = \mu_{sp0} \exp\left(\frac{t_b}{t_{sp0}}\right)$ .
- The bulk phonon–limited mobility  $\mu_{bp}$  is given by  $\mu_{bp} = P_1 \mu_{ac,1} + (1 - P_1) \mu_{ac,2}$ , where the index  $v = 1, 2$  refers to the unprimed and primed ladder. The populations of the unprimed ladder ( $P_1$ ) and the primed ladder ( $P_2 = 1 - P_1$ ) take into account the twofold and fourfold (for silicon) degeneracy. These are given by:

$$P_1 = p_1 + \frac{1 - p_1}{1 + p_2 \exp\left\{ -p_3 \left( \frac{\Delta E_C}{k_B T} \right) \right\}}$$

## Chapter 10: Mobility Models

### Perpendicular Field–Dependent Mobility Models

where  $p_1$ ,  $p_2$ , and  $p_3$  are model parameters, and  $\Delta E_C$  is the energy separation between the energy minima of the two ladders given by:

$$\Delta E_C = \left( \frac{\hbar\pi}{\sqrt{2}t_b} \right)^2 \left( \frac{1}{m_{z2}} - \frac{1}{m_{z1}} \right)$$

#### Note:

For large thicknesses,  $P_1$  is independent from the silicon thickness and barely depends on the perpendicular electric field, as expected for the bulk-limiting case. When the thickness is reduced to a few nanometers, the carriers populate more the unprimed ladder as a consequence of the increase in  $\Delta E_C$ , and the mobility increases because of the lower mass of the unprimed ladder.

The acoustic phonon–limited bulk mobility for the two ladders is given by:

$$\mu_{ac,v} = \left( \frac{W_{Tv}}{1 \text{ nm}} \right) \frac{\mu_{ac0,v}}{\left[ 1 + \left( \frac{W_{Tv}}{W_{Fv}} \right)^{\beta} \right]^{1/\beta}} \quad (157)$$

where  $W_{Tv}$  and  $W_{Fv}$  are the effective widths of the electron distribution relative to the  $v$  ladder for the two extreme cases of (i) structural-confinement dominated (small silicon thickness) and (ii) large electric field (and large silicon thickness) confinement, respectively. The effective thickness for case (i) is given by:

$$W_{Tv} = \frac{2}{3}t_b + W_{T0v} \left( \frac{t_b}{1 \text{ nm}} \right)^4 \left( \frac{F_{\perp}}{1 \text{ MV/cm}} \right) \quad (158)$$

The effective thickness for case (ii), under the assumption that the carriers confined by the strong electric field occupy only the lowest unprimed subband, is given by the Takagi model [9]:

$$W_{Fv} = W_{F0v} \left( \frac{F_{\perp}}{1 \text{ MV/cm}} \right)^{-\gamma} \quad (159)$$

Table 47 Parameters of thin-layer mobility model

Parameter symbol	Parameter name	Description	Type	Unit
A	a	Fitting parameter	float	—
$\alpha$	alpha	Fitting parameter	float	—
$\beta$	beta	Fitting parameter	float	—
$\gamma$	gamma	Fitting parameter	float	—

## Chapter 10: Mobility Models

### Perpendicular Field–Dependent Mobility Models

*Table 47 Parameters of thin-layer mobility model (Continued)*

Parameter symbol	Parameter name	Description	Type	Unit
$\delta$	delta	Fitting parameter	float	cm <sup>2</sup> /Vs
$\eta$	eta	Fitting parameter	float	V <sup>2</sup> /cms
$v$	nu	Fitting parameter	float	—
$F_{tf0}$	ftf0	Fitting parameter	float	V/cm
$l_{crit}$	lcrit	Fitting parameter	float	cm
$\mu_{ac01}$	muac01	Fitting parameter	float	cm <sup>2</sup> /Vs
$\mu_{ac02}$	muac02	Fitting parameter	float	cm <sup>2</sup> /Vs
$\mu_{sp0}$	musp0	Fitting parameter	float	cm <sup>2</sup> /Vs
$\mu_{tf0}$	mutf0	Fitting parameter	float	cm <sup>2</sup> /Vs
$m_{z1}$	mz1	First ladder mass	float	$m_0$
$m_{z2}$	mz2	Second ladder mass	float	$m_0$
$N_1$	n1	Fitting parameter	float	cm <sup>-3</sup>
$p_1$	p1	Fitting parameter	float	—
$p_2$	p2	Fitting parameter	float	—
$p_3$	p3	Fitting parameter	float	—
$t_{min}$	tmin	Fitting parameter	float	nm
$t_{sp0}$	tsp0	Fitting parameter	float	nm
$W_{f01}$	wf01	Fitting parameter	float	nm

## Chapter 10: Mobility Models

### Lateral Field–Dependent Mobility Models

Table 47 Parameters of thin-layer mobility model (Continued)

Parameter symbol	Parameter name	Description	Type	Unit
$W_{f02}$	Wf02	Fitting parameter	float	nm
$W_{t01}$	Wt01	Fitting parameter	float	nm
$W_{t02}$	Wt02	Fitting parameter	float	nm

## Changing Default Parameter Values

### Note:

See Part IV for the default parameter values for different semiconductor material models.

To change the default parameter values for this mobility model in the input file, use the following syntax:

```
material <material>.〈bandcontainer〉.Thin_Layer.<parameter> <value>
```

### Example

Set the value of  $\delta$  for electrons in silicon to  $6.0 \times 10^{14} \text{ cm}^2/\text{Vs}$ :

```
material Silicon.conduction.thin_layer.delta 6.0e14
```

---

## Lateral Field–Dependent Mobility Models

Applying a lateral field–dependent mobility model modifies the mobility to reflect high-field velocity saturation effects. The resulting mobility  $\mu$  is then the finalized mobility applied throughout the simulation domain. The following models are available:

- [No Model](#)
- [Caughey–Thomas Mobility Model](#)

---

## Calculation of the Lateral Electric Field

The electric field used for the lateral field–dependent mobility models is based on the gradient of the quasi-Fermi level. This gives a more stable solution and provides a smoother electric field than using the gradient of the electrostatic potential. Another reason for this choice is that, for variability simulations that include random discrete dopants, there are very sharp localized spikes in the electrostatic potential at the positions of the discrete dopants.

## Chapter 10: Mobility Models

### Lateral Field–Dependent Mobility Models

This results in artificial short-range fluctuations in mobility if the gradient of this electrostatic potential is used as the electric field in the field-dependent models here.

---

## No Model

Selecting `NONE` means that no lateral dependence of the electric field is accounted for, and the perpendicular field mobility remains unmodified, such that:

$$\mu = \mu_{\perp} \quad (160)$$

---

## Caughey–Thomas Mobility Model

The Caughey–Thomas mobility model [10] is an empirical fit to velocity-field characteristics and is given by:

$$\mu = \frac{(1 + \alpha)\mu_{\perp}}{\alpha + \left[ 1 + \left( \frac{(1 + \alpha)\mu_{\perp}E_{\parallel}}{v_{\text{sat}}(T)} \right)^{\beta} \right]^{1/\beta}} \quad (161)$$

where:

- $\mu_{\perp}$  is the mobility from the previously evaluated perpendicular field–dependent mobility model (see [Perpendicular Field–Dependent Mobility Models on page 323](#)).
- $E_{\parallel}$  is the field parallel to the direction of transport.
- $v_{\text{sat}}(T)$  is a temperature-dependent saturation velocity model, where the temperature-dependent saturation velocity  $v_{\text{sat}}$  is modeled following [11] as:

$$v_{\text{sat}} = v_{\text{sat}} \left( \frac{300}{T} \right)^{v_{\text{exp}}}$$

- $\beta$  is a fitting parameter that is modeled with temperature dependence as

$$\beta = \beta_0 \left( \frac{T}{300} \right)^{\beta_{\text{exp}}}.$$

Table 48 Parameters of Caughey–Thomas mobility model as defined in [Equation 161](#)

Parameter symbol	Parameter name	Description	Type	Unit
$v_{\text{sat}}$	<code>vsat</code>	Saturation velocity	float	cm/s
$v_{\text{exp}}$	<code>vexp</code>	Fitting parameter	float	–
$\beta_0$	<code>beta0</code>	Fitting parameter	float	–

## Chapter 10: Mobility Models

### Ballistic Mobility Models

Table 48 Parameters of Caughey–Thomas mobility model as defined in [Equation 161](#)

Parameter symbol	Parameter name	Description	Type	Unit
$\beta_{\text{exp}}$	bexp	Fitting parameter	float	–
$\alpha$	alpha	Fitting parameter	float	–

## Changing Default Parameter Values

### Note:

See Part IV for the default parameter values for different semiconductor material models.

To change the default parameter values for this mobility model in the input file, use the following syntax:

```
material <material>.<bandcontainer>.Caughey.<parameter> <value>
```

### Example

Set the value of  $v_{\text{sat}}$  for electrons in silicon to  $1.8 \times 10^7$  cm/s:

```
material Silicon.conduction.caughey.vsat 1.8e7
```

---

## Ballistic Mobility Models

You can introduce an effective *ballistic* mobility to mimic ballistic effects as the channel length is scaled. The following models are available:

- [No Model](#)
- [Shur Mobility Model](#)

---

### No Model

Selecting `NONE` means that no ballistic model is accounted for, and the final mobility remains unmodified, such that:

$$\mu = \mu_{\text{final}} \tag{162}$$

## Chapter 10: Mobility Models

### Ballistic Mobility Models

---

## Shur Mobility Model

The Shur mobility model [12] is an approach to model the effective ballistic mobility and is given by:

$$\mu_{\text{ball}} = \frac{2qL}{\pi m v_{\text{th}}} \quad (163)$$

where:

- $L$  is the device length.
- $m$  is the effective mass.
- $v_{\text{th}}$  is the thermal velocity model, where the thermal velocity  $v_{\text{th}}$  is modeled following [12] as  $v_{\text{th}} = \left(\frac{8kT}{\pi m}\right)^{1/2}$ .

Table 49 Parameters of Shur mobility model as defined in Equation 163

Parameter symbol	Parameter name	Description	Type	Unit
$v_{\text{th}}$	vth	Thermal velocity	float	cm/s
$L$	lchan	Channel length	float	nm
$m$	m	Effective mass	float	—

## Changing Default Parameter Values

### Note:

See Part IV for the default parameter values for different semiconductor material models.

To change the default parameter values for this mobility model in the input file, use the following syntax:

```
material <material>.bandcontainer.shur.<parameter> <value>
```

### Example

Set the value of  $v_{\text{th}}$  for electrons in silicon to  $1.8 \times 10^7$  cm/s:

```
material Silicon.conduction.shur.vth 1.8e7
```

---

## Strain-Dependent Mobility Models

Applying a strain-dependent mobility model acts to capture the impact of stress-induced band-structure modifications on the low-field carrier mobility. The following models are available:

- No Model
- Simple Strain Enhancement Mobility Model
- Multivalley Mobility Model

---

### No Model

Selecting `NONE` means that no stress effect on mobility is accounted for, and the final mobility remains unmodified, such that:

$$\mu = \mu_0 \quad (164)$$

---

### Simple Strain Enhancement Mobility Model

The simple strain enhancement (SSE) mobility model provides a simple analytic expression that enhances or reduces the low-field mobility based on the value of the strain at the mesh node. This is an anisotropic model, so the strain component in each of the Cartesian directions is used to modify the mobility in that direction.

The strain enhancement factor,  $\beta$ , is defined for electrons with the following expression:

$$\beta = \begin{cases} 1 + R^+ \left( 1 - \exp \left[ -\frac{\varepsilon}{\tau} \right] \right) & \varepsilon \geq 0 \\ 1 - R^- \left( 1 - \exp \left[ \frac{\varepsilon}{\tau'} \right] \right) & \varepsilon < 0 \end{cases} \quad (165)$$

where:

- $\varepsilon$  is the local strain.
- $R^+ = \beta_{\max} - 1$  and  $R^- = 1 - \beta_{\min}$ .
- $\tau' = \tau \times \frac{R^-}{R^+}$ .

For hole mobility, the sign of the strain is inverted, so that negative strain gives mobility enhancement and positive strain gives mobility reduction.

## Chapter 10: Mobility Models

### Strain-Dependent Mobility Models

The  $\beta$  parameter is then used to scale the  $\mu_{\max}$  parameter in low-field mobility models (such as Masetti and Philips), which provides the mobility enhancement to the low-field mobility, that is:

$$\mu'_{\max} = \beta \times \mu_{\max} \quad (166)$$

By default, the strain enhancement factor,  $\beta$ , also scales the saturation velocity,  $v_{\text{sat}}$ , used in the Caughey–Thomas mobility model (see [Caughey–Thomas Mobility Model on page 331](#)). The degree to which  $\beta$  affects  $v_{\text{sat}}$  can be set with the saturation velocity factor,  $\alpha$ , which takes a value in the range  $0 \leq \alpha \leq 1$ :

- If  $\alpha = 0$ , then  $v_{\text{sat}}$  is not scaled.
- If  $\alpha = 1$ , which is the default value, then  $v_{\text{sat}}$  is scaled by the full value of  $\beta$ .

A value between 0 and 1 scales the applied scaling factor linearly from 1 to  $\beta$ , that is:

$$v'_{\text{sat}} = v_{\text{sat}} \times (1 + \alpha(\beta - 1)) \quad (167)$$

Table 50 Parameters of SSE mobility model with default parameter values

Parameter symbol	Parameter name	Description	Default		Unit
			Electrons	Holes	
$\beta_{\max}$	max_factor	Maximum mobility enhancement factor	35.0	3.7	–
$\beta_{\min}$	min_factor	Minimum mobility reduction factor	0.1	0.25	–
$\tau$	tau	Strain coefficient	0.25	0.3	–
$v_{\text{sat}}$	vsat_factor	Saturation velocity factor	1.0	1.0	–

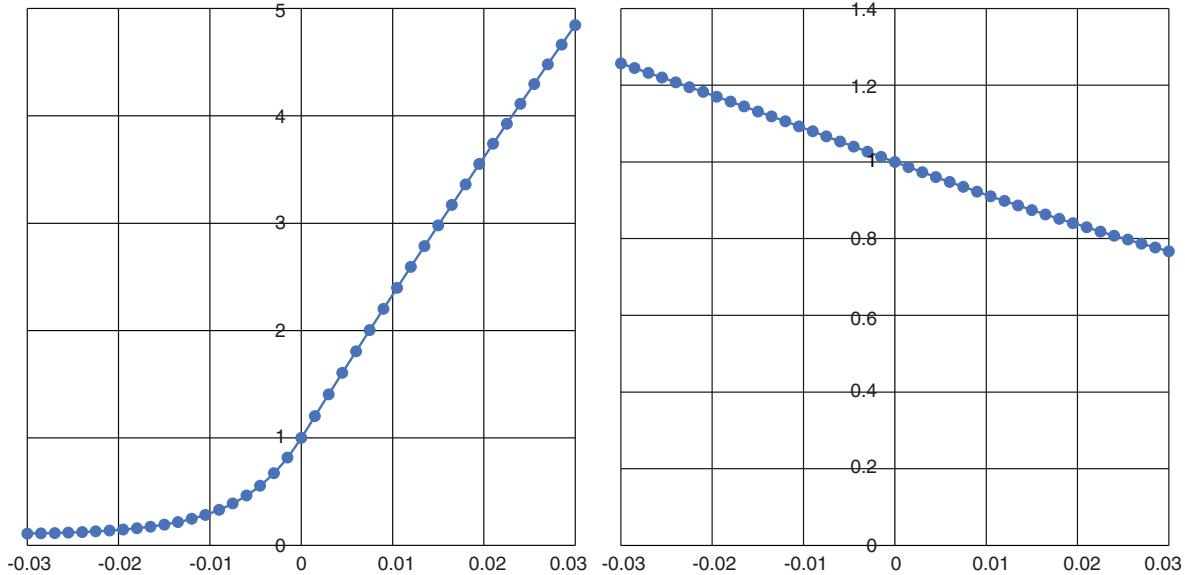
## Changing Default Parameter Values

To change the default parameter values, listed in [Table 50](#), use the following syntax in the input file:

```
material <material>.<bandcontainer>.sse.<parameter> <value>
```

[Figure 38](#) shows the default values of the strain enhancement factor,  $\beta$ , for electrons and holes. These default values have been set to produce a similar enhancement to the first-order piezoresistance mobility model available in Sentaurus Device.

**Figure 38** Strain enhancement factor,  $\beta$ , as a function of strain with default parameter values for (left) electrons and (right) holes



## Multivalley Mobility Model

This model captures the impact of both mass modification and valley splitting resulting from the application of stress. Following [13], the mean free time between collisions is assumed to be constant (applied to both electrons and holes in this case). So for a given direction in the device frame (x, y, or z), the mobility is estimated as:

$$\mu = \sum_{i=1}^{\text{valleys}} \frac{f_i}{m_{C,i}} \quad (168)$$

where:

- $m_C$  is the effective conductivity mass.
- $f_i$  is the occupation of valley  $i$  as a fraction of all valleys (this allows the impact of valley splitting to be accounted for).

For electrons, the modification of mass follows [14]. For holes, it is extracted from the six-band k·p calculation at the thermal energy level.

This mobility is calculated for a given material both with and without stress applied, so the resulting mobility is calculated as:

$$\mu = \frac{\mu_{\text{stressed}}}{\mu_{\text{relaxed}}} \mu_0 \quad (169)$$

## Chapter 10: Mobility Models

### References

where  $\mu_0$  is the low-field mobility as calculated by the bulk mobility model.

By default, values for the effective mass are calculated using the internal model, but you can overwrite them in the input file.

**Table 51** lists the parameters of the model. These masses must be modified on a valley-by-valley basis rather than by the model itself.

*Table 51 Parameters of multivalley mobility model*

Parameter symbol	Parameter name	Description	Type	Unit
$m_{C,x}$	<code>mx0</code>   <code>mxS</code>	Conductivity mass in the x-direction relaxed and stressed	float	–
$m_{C,y}$	<code>my0</code>   <code>myS</code>	Conductivity mass in the y-direction relaxed and stressed	float	–
$m_{C,z}$	<code>mz0</code>   <code>mzS</code>	Conductivity mass in the z-direction relaxed and stressed	float	–

## Changing Default Parameter Values

### Note:

Default parameter values are derived internally.

To change the default parameter values, use the following syntax in the Garand input file:

```
material <material>.bandcontainer.multiparameter <value>
```

### Example

Set the stressed conductivity mass along the x-direction in the X1 valley of silicon to 0.12:

```
material Silicon.conduction.X1.mxS 0.12
```

---

## References

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## Chapter 10: Mobility Models

### References

- [3] C. Lombardi *et al.*, “A Physically Based Mobility Model for Numerical Simulation of Nonplanar Devices,” *IEEE Transactions on Computer-Aided Design*, vol. 7, no. 11, pp. 1164–1171, 1988.
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- [5] B. K. Ridley, *Quantum Processes in Semiconductors*, Oxford: Clarendon Press, 4th ed., 1999.
- [6] K. Yamaguchi, “Field-Dependent Mobility Model for Two-Dimensional Numerical Analysis of MOSFET’s,” *IEEE Transactions on Electron Devices*, vol. ED-26, no. 7, pp. 1068–1074, 1979.
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- [9] S. Takagi *et al.*, “On the Universality of Inversion Layer Mobility in Si MOSFET’s: Part II—Effects of Surface Orientation,” *IEEE Transactions on Electron Devices*, vol. 41, no. 12, pp. 2363–2368, 1994.
- [10] D. M. Caughey and R. E. Thomas, “Carrier Mobilities in Silicon Empirically Related to Doping and Field,” *Proceedings of the IEEE*, vol. 55, no. 12, pp. 2192–2193, 1967.
- [11] C. Canali *et al.*, “Electron and Hole Drift Velocity Measurements in Silicon and Their Empirical Relation to Electric Field and Temperature,” *IEEE Transactions on Electron Devices*, vol. ED-22, no. 11, pp. 1045–1047, 1975.
- [12] M. S. Shur, “Low Ballistic Mobility in Submicron HEMTs,” *IEEE Electron Device Letters*, vol. 23, no. 9, pp. 511–513, 2002.
- [13] B. Obradovic *et al.*, “A Physically-Based Analytic Model for Stress-Induced Hole Mobility Enhancement,” *Journal of Computational Electronics*, vol. 3, no. 3–4, pp. 161–164, 2004.
- [14] E. Ungersboeck *et al.*, “The Effect of General Strain on the Band Structure and Electron Mobility of Silicon,” *IEEE Transactions on Electron Devices*, vol. 54, no. 9, pp. 2183–2190, 2007.

# 11

## Scattering Mechanisms

---

This chapter describes the scattering rate models used to define carrier transport in Monte Carlo simulations. These models and their applications apply equally to carrier transport in conduction bands and valence bands, although default model parameter values differ in each case.

---

### Scattering Rate Tabulation

Scattering rates are tabulated for carriers in each minima associated with each band in each semiconductor material's conduction and valence band containers. Tabulation stores scattering rates as a function of carrier energy up to a maximum energy  $E_{\max}$  within the band and considering an energy resolution. The energy resolution defines the number of uniform energy bins between 0 and  $E_{\max}$ .

Table 52 Parameters for defining scattering rate tabulation

Parameter symbol	Parameter name	Description	Type	Unit
$E_{\max}$	E	Sets the maximum energy.	float	eV
$\Delta E$	dE	Sets the energy resolution.	float	eV

See [Default Semiconductor Materials on page 381](#) for scattering rates for each semiconductor material model.

---

### Changing Default Parameter Values

To change the default energy range of the scattering rate tabulation in the input file, use the following syntax:

```
material <material>.bandcontainer.<band>.<valley>.rates.<parameter>
<value>
```

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### Elastic Acoustic Phonon Scattering

where:

- <material> is the name of a semiconductor material.
- <bandcontainer> is either conduction or valence.
- <band> is the name of a band in the band container.
- <valley> is the unique name of a local minimum within the specified band.
- <parameter> is the name of a parameter listed in [Table 52 on page 339](#).
- <value> is the new value of the parameter, specified with the expected type.

#### Example

Define scattering rates in the silicon conduction band X1 valley to be tabulated up to an energy of 2.0 eV with a resolution of 2 meV:

```
material silicon.conduction.C1.X1.rates.E 2.0
material silicon.conduction.C1.X1.dE      2.0e-3
```

---

## Elastic Acoustic Phonon Scattering

Elastic carrier scattering from acoustic phonons within the equipartition approximation defines the parameters listed in [Table 53](#).

*Table 53 Parameters for defining elastic acoustic phonon scattering*

Parameter symbol	Parameter name	Description	Type	Unit
D	D	Sets the deformation potential of the scattering.	float	eV
v	v	Sets the dispersion sound velocity used to approximate the linear dispersion near the zone center.	float	m/s
Final valley	final	Specifies the name of the final valley for scattering (should assume intravalley scattering).	string	–

See [Default Semiconductor Materials on page 381](#) for deformation potentials and sound velocities for elastic acoustic phonon mechanisms.

## Chapter 11: Scattering Mechanisms

### Inelastic Acoustic Phonon Scattering

---

## Changing Default Parameter Values

To change the default parameter values of the scattering mechanism in the input file, use the following syntax:

```
material
<material>.<bandcontainer>.<band>.<valley>.<mechanism>.<parameter>
<value>
```

where:

- <material> is the name of a semiconductor material.
- <bandcontainer> is either conduction or valence.
- <band> is the name of a band in the band container.
- <valley> is the name of a local minimum within the specified band.
- <mechanism> is the name of an elastic acoustic phonon scattering mechanism in the band.
- <parameter> is the name of a parameter listed in [Table 53](#).
- <value> is the new value of the parameter, specified with the expected type.

### Example

Set the deformation potential (6.0 eV) and sound velocity (5000 m/s) for the acoustic phonon mechanism within the X1 valley of the InGaAs conduction band:

```
material InGaAs.conduction.C1.X1.Ac.D 6.0
material InGaAs.conduction.C1.X1.Ac.v 5.0e3
```

---

## Inelastic Acoustic Phonon Scattering

Inelastic carrier scattering from acoustic phonons defines the parameters listed in [Table 54](#).

*Table 54 Parameters for defining inelastic acoustic phonon scattering*

Parameter symbol	Parameter name	Description	Type	Unit
D	D	Sets the deformation potential of the scattering.	float	eV
v	v	Sets the sound velocity used to approximate the linear dispersion near the zone center.	float	m/s

## Chapter 11: Scattering Mechanisms

### Inelastic Acoustic Phonon Scattering

Table 54 Parameters for defining inelastic acoustic phonon scattering (Continued)

Parameter symbol	Parameter name	Description	Type	Unit
c	c	Sets the coefficient used to fit the phonon dispersion to a quadratic approximation.	float	$\text{m}^2/\text{s}$
Final valley	final	Sets the name of the final valley for scattering (should assume intravalley scattering).	string	—

See [Default Semiconductor Materials on page 381](#) for the deformation potentials, sound velocities, and quadratic fitting for inelastic acoustic phonon scattering mechanisms.

---

## Changing Default Parameter Values

To change the default parameter values in the input file, use the following syntax:

```
material  
<material>. <bandcontainer>. <band>. <valley>. <mechanism>. <parameter>  
<value>
```

where:

- <material> is the name of a semiconductor material.
- <bandcontainer> is either conduction or valence.
- <band> is the name of a band in the band container.
- <valley> is the name of a local minimum within the specified band.
- <mechanism> is the name of an inelastic acoustic phonon scattering mechanism in the band.
- <parameter> is the name of a parameter listed in [Table 54](#).
- <value> is the new value of the parameter, specified with the expected type.

### Example

Set the deformation potential (3.0 eV), the longitudinal sound velocity (8000 m/s), and the fitting ( $-1.5 \times 10^{-7} \text{ m}^2/\text{s}$ ) for the inelastic longitudinal acoustic phonon scattering mechanism within the X1 valley of the silicon conduction band:

```
material silicon.conduction.C1.X1.Acl.D 3.0  
material silicon.conduction.C1.X1.Acl.v 8.0e3  
material silicon.conduction.C1.X1.Acl.c -1.5e-7
```

## Chapter 11: Scattering Mechanisms

### Optical Phonon Scattering

---

## Optical Phonon Scattering

Inelastic carrier scattering from dispersionless optical phonon defines the parameters in [Table 55](#).

*Table 55 Parameters for defining optical phonon scattering*

Parameter symbol	Parameter name	Description	Type	Unit
$E_{\text{op}}$	E	Sets the optical phonon energy.	float	eV
$D_{\text{op}}$	cc	Sets the coupling constant for optical phonon scattering.	float	eV/m
Final valley	final	Sets the name of the final valley for scattering.	string	—

See [Default Semiconductor Materials on page 381](#) for phonon energies and coupling constant for optical phonon mechanisms.

---

## Changing Default Parameter Values

To change the default parameter values in the input file, use the following syntax:

```
material
<material>.bandcontainer.<band>.<valley>.<mechanism>.<parameter>
<value>
```

where:

- `<material>` is the name of a semiconductor material.
- `<bandcontainer>` is either `conduction` or `valence`.
- `<band>` is the name of a band in the band container.
- `<valley>` is the name of a local minimum within the specified band.
- `<mechanism>` is the name of an optical phonon scattering mechanism within the band.
- `<parameter>` is the name of a parameter listed in [Table 55](#).
- `<value>` is the new value of the parameter, specified with the expected type.

## Chapter 11: Scattering Mechanisms

### Polar-Optical Phonon Scattering

#### Example

Set the optical phonon energy (15.0 meV) and the coupling constant ( $8 \times 10^9$  eV/m) for the g1x2 optical phonon scattering mechanism within the silicon conduction band X1 valley, and declare the final valley to be the X2 valley within the same conduction band:

```
material silicon.conduction.C1.X1.g1X2.E      15.0e-3
material silicon.conduction.C1.X1.g1X2.cc     8.0e9
material silicon.conduction.C1.X1.g1X2.final X2
```

---

## Polar-Optical Phonon Scattering

Inelastic carrier scattering from dispersionless polar-optical phonon defines the parameters in [Table 56](#).

*Table 56 Parameters for defining polar-optical phonon scattering*

Parameter symbol	Parameter name	Description	Type	Unit
$E_{op}$	E	Sets the polar-optical phonon energy.	float	eV
Final valley	final	Sets the name of the final valley for scattering.	string	-
Scattering rate	rate	Specifies how the rate should be tabulated. Options are: <ul style="list-style-type: none"><li>• average</li><li>• maximum</li></ul>	string	-

See [Default Semiconductor Materials on page 381](#) for phonon energies for polar optical phonon scattering mechanisms.

---

## Changing Default Parameter Values

To change default parameter values in the input file, use the following syntax:

```
material
<material>. <bandcontainer>. <band>. <valley>. <mechanism>. <parameter>
<value>
```

where:

- <material> is the name of a semiconductor material.
- <bandcontainer> is either `conduction` or `valence`.

## Chapter 11: Scattering Mechanisms

### Ionized Impurity Scattering

- <band> is the name of a band in the band container.
- <valley> is the name of a local minimum within the specified band.
- <mechanism> is the name of a polar-optical phonon scattering mechanism in the band.
- <parameter> is the name of a parameter listed in [Table 56](#).
- <value> is the new value of the parameter, specified with the expected type.

#### Example

Set the polar-optical phonon energy for the polar-optical phonon scattering mechanism in the InGaAs conduction band G-valley to 25.0 meV, and declare the final valley to be the G-valley within the same conduction band:

```
material ingaas.conduction.C2.G.pop.E      25.0e-3
material ingaas.conduction.C2.G.pop.final G
```

---

## Ionized Impurity Scattering

Elastic carrier scattering from ionized impurities defines the parameters in [Table 57](#).

*Table 57 Parameters for defining ionized impurity scattering*

Parameter symbol	Parameter name	Description	Type	Unit
Model	model	Specifies the name of the model of ionized impurity scattering to use. Options are: <ul style="list-style-type: none"><li>• BH for the Brooks–Herring model</li><li>• TBE for Ridley’s third-body exclusion model</li></ul>	string	–
Final valley	final	Specifies the name of the final valley for scattering (should assume intravalley scattering).	string	–
Screening	screening	Specifies the screening approach for ionized impurity scattering. Options are: <ul style="list-style-type: none"><li>• dynamic (for Brooks–Herring model only)</li><li>• static</li></ul>	string	–

## Chapter 11: Scattering Mechanisms

### Ionized Impurity Scattering

Table 57 Parameters for defining ionized impurity scattering (Continued)

Parameter symbol	Parameter name	Description	Type	Unit
Correction	correction	Specifies whether to apply the calibrated correction term to the impurity scattering model that allows for experimental mobility to be recovered. This parameter allows it to be deactivated. Options are: <ul style="list-style-type: none"><li>• off</li><li>• on</li></ul>	string	–

See [Default Semiconductor Materials on page 381](#) for the default ionized impurity model for different semiconductors.

---

## Changing Default Parameter Values

To change the default parameter values in the input file, use the following syntax:

```
material  
<material>. <bandcontainer>. <band>. <valley>. <mechanism>. <parameter>  
<value>
```

where:

- <material> is the name of a semiconductor material.
- <bandcontainer> is either conduction or valence.
- <band> is the name of a band in the band container.
- <valley> is the name of a local minimum within the specified band.
- <mechanism> is the name of an ionized impurity scattering mechanism in the band.
- <parameter> is the name of a parameter listed in [Table 57](#).
- <value> is the new value of the parameter, specified with the expected type.

### Example

Define the ionized impurity scattering model within the silicon conduction band X1 valley to be Brooks–Herring with dynamic screening and no correction term:

```
material silicon.conduction.C1.X1.II.model      BH  
material silicon.conduction.C1.X1.II.screening  dynamic  
material silicon.conduction.C1.X1.II.correction off
```

## Chapter 11: Scattering Mechanisms

### Surface Roughness Scattering

---

## Surface Roughness Scattering

Elastic carrier scattering from rough interfaces defines the parameters in [Table 58](#).

*Table 58 Parameters for defining surface roughness scattering*

Parameter symbol	Parameter name	Description	Type	Unit
Model	model	Sets the name of the stochastic surface roughness model to use. Only option is <code>Ando</code> .	string	—
Final valley	final	Sets the name of the final valley for scattering (should assume intravalley scattering).	string	—
Field limit	effective_field_limit	Sets a limit to the effective field for calculating the scattering rate. This can also be done on a per-material basis.	float	MV/cm

See [Default Semiconductor Materials on page 381](#) for the default surface roughness model for different semiconductors.

---

## Changing Default Parameter Values

To change the default parameter values in the input file, use the following syntax:

```
material
<material>.〈bandcontainer〉.〈band〉.〈valley〉.〈mechanism〉.〈parameter〉
<value>
```

where:

- `<material>` is the name of a semiconductor material.
- `<bandcontainer>` is either `conduction` or `valence`.
- `<band>` is the name of a band in the band container.
- `<valley>` is the name of a local minimum within the specified band.
- `<mechanism>` is the name of a surface roughness scattering mechanism in the band.
- `<parameter>` is the name of a parameter listed in [Table 58](#).
- `<value>` is the new value of the parameter, specified with the expected type.

## Chapter 11: Scattering Mechanisms

### Remote Coulomb Scattering

#### Examples

Define the surface roughness scattering model as Ando within the silicon conduction band X1 valley:

```
material silicon.conduction.C1.X1.SR.model Ando
```

Set the limit of the effective field to 2.5 MV/cm:

```
material silicon.valence.HH.vhh.SR.effective_field_limit 2.5
```

Modify the field limit for all bands or valleys in a given material:

```
material silicon.effective_field_limit 6.5
```

---

## Remote Coulomb Scattering

Parameters for elastic scattering from interface charges are defined in [Table 59](#).

*Table 59 Parameters for defining remote Coulomb scattering*

Parameter symbol	Parameter name	Description	Type	Unit
Final valley	final	Sets the name of the final valley for scattering (should assume intravalley scattering).	string	–
$z_d$	zd	Sets the depth of the charge centroid.	float	nm
$E_0$	e0	Sets the minimum energy for the tabulating rate.	float	eV
$N_0$	n0	Sets the minimum screening density.	float	$\text{cm}^{-3}$

See [Default Semiconductor Materials on page 381](#) for the remote Coulomb model for different semiconductors.

---

## Changing Default Parameter Values

To change the default parameter values in the input file, use the following syntax:

```
material  
<material>. <bandcontainer>. <band>. <valley>. <mechanism>. <parameter>  
<value>
```

## Chapter 11: Scattering Mechanisms

### Alloy Scattering

where:

- <material> is the name of a semiconductor material.
- <bandcontainer> is either conduction or valence.
- <band> is the name of a band in the band container.
- <valley> is the name of a local minimum within the specified band.
- <mechanism> is the name of a remote Coulomb scattering mechanism in the band.
- <parameter> is the name of a parameter listed in [Table 59](#).
- <value> is the new value of the parameter, specified with the expected type.

### Examples

Define the depth of the centroid to 1 nm within the silicon conduction band X1 valley:

```
MATERIAL Silicon.conduction.C1.X1.RC.Zd 1.0
```

Set the minimum energy for the tabulating rate to 0.1 eV:

```
MATERIAL Silicon.conduction.C1.X1.RC.E0 0.1
```

Set the minimum screening density to  $5 \times 10^{17} \text{ cm}^{-3}$ :

```
MATERIAL Silicon.conduction.C1.X1.RC.NO 5.d-17
```

---

## Alloy Scattering

Elastic carrier scattering from alloy potential differences defines the parameters in [Table 60](#).

*Table 60 Parameters for defining alloy scattering*

Parameter symbol	Parameter name	Description	Type	Unit
$U$	U	Sets the alloy scattering potential to use.	float	eV
Final valley	final	Sets the name of the final valley for scattering (should assume intravalley scattering).	string	—

See [Default Semiconductor Materials on page 381](#) for the default alloy scattering model for different semiconductors.

## Chapter 11: Scattering Mechanisms

### Impact Ionization: Keldysh Model

---

## Changing Default Parameter Values

To change default parameter values in the input file, use the following syntax:

```
material  
<material>.<bandcontainer>.<band>.<valley>.<mechanism>.<parameter>  
<value>
```

where:

- <material> is the name of a semiconductor material.
- <bandcontainer> is either conduction or valence.
- <band> is the name of a band in the band container.
- <valley> is the name of a local minimum within the specified band.
- <mechanism> is the name of an alloy scattering mechanism in the band.
- <parameter> is the name of a parameter listed in [Table 60](#).
- <value> is the new value of the parameter, specified with the expected type.

### Example

Set the alloy scattering potential to 1.0 eV within the Si<sub>50</sub>Ge<sub>50</sub> conduction band X1 valley:

```
material si50ge50.conduction.C1.X1.al.U 1.0
```

---

## Impact Ionization: Keldysh Model

You can implement impact ionization by using the empirical analytic Keldysh model. Like all mechanisms, it must be defined within an existing valley definition, by using the following general syntax:

```
define <material>.<bandcontainer>.<band>.<valley>.<mechanism> KeldyshII
```

where:

- <material> is the name of a semiconductor material.
- <bandcontainer> is either conduction or valence.
- <band> is the name of a band in the band container.
- <valley> is the name of a valley within the specified band.
- <mechanism> is the user-defined name to be associated with the new impact ionization mechanism. It must be unique among the other mechanisms defined within the named valley.

## Chapter 11: Scattering Mechanisms

### Impact Ionization: Keldysh Model

For example, the following input file command defines a new impact ionization mechanism called `ImpI` in the default X1 valley of the silicon conduction band:

```
define Silicon.conduction.C1.X1.ImpI KeldyshII
```

After it is defined, you can assign the mechanism model parameters by using the `material` command.

*Table 61 Parameters for defining impact ionization using Keldysh model*

Parameter symbol	Parameter name	Description	Type	Unit
$\Lambda$	L	Sets the energy-dependent coefficient.	float	$\text{ps}^{-1}$
$E_t$	Et	Sets the threshold energy.	float	eV
$\gamma$	g	Sets the energy-dependent power.	float	—
Final valley	final	Sets the name of the final valley for scattering.	string	—

Both  $\Lambda$  and  $\gamma$  are user-defined tables of values as a function of energy that support interpolation between defined values (see [Interpolation Methods on page 301](#)).

---

## Scattering Rate

The scattering rate as a function of energy for carriers within the valley in which the mechanism is defined is given as:

$$\Gamma(E) = \Lambda(E) \left( \frac{E - E_t}{E_t} \right)^{\gamma(E)} \quad (170)$$

The threshold energy for the onset of impact ionization defaults to the material bandgap,  $E_g$ , unless you specify the threshold energy in the scattering mechanism definition. The parameters  $\Lambda$  and  $\gamma$  are, in general, functions of energy that are defined as piecewise interpolated tables.

---

## State After Scattering

The energies of the initial and the secondary carrier after scattering are defined simply as  $E' = (E - E_t)/3$ , where the excess energy above the threshold energy is divided equally among the final three carriers.

## Chapter 11: Scattering Mechanisms

### Impact Ionization: Kane Random-k Approximation Model

The initial state of the carrier after scattering is restricted to the final valley named in the mechanism definition. For example:

```
material Silicon.conduction.C1.X1.ImpI.final X2
```

The secondary carriers are randomly assigned bands or valleys weighted by the available densities-of-states. The momentum of the initial carrier and both secondary carriers is isotropically oriented, consistent with the final energy.

---

## Impact Ionization: Kane Random-*k* Approximation Model

You can implement impact ionization by using the Kane random-*k* approximation (RKA) model [1]. Like all mechanisms, it must be defined within an existing valley definition, by using the following general syntax:

```
define <material>.<bandcontainer>.<band>.<valley>.<mechanism> KaneII
```

where:

- <material> is the name of a semiconductor material.
- <bandcontainer> is either conduction or valence.
- <band> is the name of a band in the band container.
- <valley> is the name of a valley within the specified band.
- <mechanism> is the user-defined name to be associated with the new impact ionization mechanism. It must be unique among the other mechanisms defined within the named valley.

For example, the following input file command defines a new impact ionization mechanism called ImpI in the default X1 valley of the silicon conduction band:

```
define Silicon.conduction.C1.X1.ImpI KaneII
```

After it is defined, you can assign the mechanism model parameters by using the `material` command.

Table 62 Parameters for defining impact ionization using Kane RKA model

Parameter symbol	Parameter name	Description	Type	Unit
$\Lambda$	L	Sets the energy-dependent coefficient. This parameter is a user-defined table of values as a function of energy that supports interpolation between defined values (see <a href="#">Interpolation Methods on page 301</a> ).	float	$\text{nm}^9 \text{eVps}^{-1}$

## Chapter 11: Scattering Mechanisms

Backward Compatibility: Hole Scattering

Table 62 Parameters for defining impact ionization using Kane RKA model (Continued)

Parameter symbol	Parameter name	Description	Type	Unit
$dE$	<code>dE</code>	Sets the energy interval for numeric integration. Default: 1 meV	float	eV
Final valley	<code>final</code>	Sets the name of the final valley for scattering.	string	—

---

## Scattering Rate

The scattering rate as a function of energy for carriers within the valley in which the mechanism is defined is given as:

$$\Gamma(E) = \Lambda(E) \int g(E_2)g(E_3)g(E_4)dE_2dE_3 \quad (171)$$

where:

- $E$  is the energy of the incident electron (or hole).
- $E_2$  and  $E_3$  are the final electron (or hole) energies, and  $E_4$  is the final hole (or electron) energy, such that  $E = E_2 + E_3 - E_4$ .
- $g(E_2)$  and  $g(E_3)$  are the conduction (or valence) band densities-of-states at  $E_2$  and  $E_3$ , respectively.
- $g(E_4)$  is the valence (or conduction) band density-of-states at  $E_4$ .

Integration is performed numerically using a discrete energy interval  $dE$ , which has a default value of 1 meV that you can redefine.

---

## State After Scattering

The same approximation as used in the Keldysh model is used in the Kane RKA model to define the states after scattering (see [State After Scattering on page 351](#)).

---

## Backward Compatibility: Hole Scattering

The default behavior for selecting the final state after scattering has changed to improve both the calibration to measurement data and efficiency.

## Chapter 11: Scattering Mechanisms

### References

To revert to earlier behavior, use the following commands:

```
SIMULATION scattering_ave_DoS      = off
SIMULATION scattering_correction = on
SIMULATION approx_screening       = on
```

where:

- The first command deactivates the use of a spherically averaged value of the density-of-states.
- The second command reactivates a correction to the final state during the rejection loop.
- The third command activates an approximation for the screening length.

**Note:**

Use these commands with the `--compatible` command-line option to recover the appropriate parameter set (see [Parameter Compatibility on page 191](#)).

---

## References

- [1] E. O. Kane, "Electron Scattering by Pair Production in Silicon," *Physical Review*, vol. 159, no. 3, pp. 624–631, 1967.

# 12

## Scattering Models

---

*This chapter describes the carrier scattering models implemented in Garand MC.*

All models are based on first-order perturbation theory as described by Fermi's golden rule and are applied, in general, to either an analytic valley model or a full-band model (see [Analytic Valley Model on page 356](#) and [Six-Band  \$k \cdot p\$  Model on page 357](#)).

The general approach to scattering is outlined first to highlight underlying assumptions within the models, followed by specific applications to all available scattering processes, for the analytic valley model, the full-band model, and the six-band  $k \cdot p$  model.

---

### General Scattering Model

This section discusses the general scattering model.

---

### Transition Rate: Fermi's Golden Rule

All scattering is treated following first-order perturbation theory as governed by Fermi's golden rule, which states the transition rate  $S(\mathbf{k}, \mathbf{k}')$ , defining the probability per unit time of scattering from an initial state with crystal momentum  $\hbar\mathbf{k}$  to a final state with crystal momentum  $\hbar\mathbf{k}'$  as [1]:

$$S(\mathbf{k}, \mathbf{k}') = \frac{2\pi}{\hbar} |M_{\mathbf{k}', \mathbf{k}}|^2 \delta[\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}) \mp \Delta\varepsilon(\mathbf{q})] \delta_{\mathbf{k}', \mathbf{k} \pm \mathbf{q}} \quad (172)$$

where  $M_{\mathbf{k}', \mathbf{k}}$  is the matrix element that defines the coupling between states. The delta function expresses conservation of energy between the initial and final states  $\varepsilon(\mathbf{k})$  and  $\varepsilon(\mathbf{k}')$ , accounting for absorption or emission of energy  $\Delta\varepsilon(\mathbf{q})$  that is, in general, dependent on the momentum transfer  $\mathbf{q}$ , and the Kronecker delta expresses momentum conservation.

## Chapter 12: Scattering Models

### General Scattering Model

## Matrix Element

When applied to carriers in an infinite periodic lattice, the matrix element can be defined as [1]:

$$M_{k', k} = I(k, k') U_S(k - k') \quad (173)$$

where  $I(k, k')$  is the overlap integral, defined as:

$$I(k, k') = \int_{\text{cell}} u_{k'}^*(r) u_k(r) dr \quad (174)$$

and where  $u_k$  is the cell periodic part of the Bloch wavefunction [2].  $U_S(k - k')$  is defined as:

$$U_S(k - k') = \int_{-\infty}^{\infty} e^{-ik' \cdot r} U_S(r) e^{ik \cdot r} d^3 r \quad (175)$$

where  $U_S(r)$  is the mechanism-specific scattering potential as a function of real space  $r$ .

---

## Scattering Rate

Given the transition rate (Equation 172), the total scattering rate associated with an initial state  $k$  is defined as the sum over all final states  $k'$  as:

$$\Gamma(k) = \sum_{k'} S(k, k') = \frac{\Omega}{8\pi^3} \int_{k'} S(k, k') d^3 k \quad (176)$$

This assumes a quasi-continuous distribution of states in three dimensions and that carrier spin is preserved during scattering, restricting the number of final available states.

## Analytic Valley Model

The semiconductor conduction band model is defined as a multivalley approximation [2], where each valley is modeled as an ellipsoidal nonparabolic equienergy surface in  $k$ -space (see [Analytic Valley Model on page 293](#)).

For the purpose of all scattering rate calculations, analytic valleys are described as spherical equienergy surfaces. These are related to the ellipsoidal model using the Herring–Vogt transformation [3]. Integration over all final states is then performed by exploiting the spherical symmetry as:

$$\Gamma(k) = \frac{\Omega}{8\pi^3} \int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta \int_0^\infty k'^2 S(k, k') dk' \quad (177)$$

The overlap integral, included within the transition rate  $S(k, k')$ , is approximated as a constant for electron scattering by nonpolar mechanisms. This can be taken to be unity or a constant value, to be calibrated as part of the coupling with the scattering potential as in the

## Chapter 12: Scattering Models

### General Scattering Model

case of intervalley optical phonon scattering where the approximation arises due to the relatively small range of scattering angles involved [2].

For polar mechanisms, an approximation for the overlap integral is taken as [4]:

$$I(\mathbf{k}, \mathbf{k}') = \frac{[(1 + \alpha\epsilon)^{1/2}(1 + \alpha\epsilon')^{1/2} + \alpha(\epsilon\epsilon')^{1/2}\cos\theta]^2}{(1 + 2\alpha\epsilon)(1 + 2\alpha\epsilon')} \quad (178)$$

where  $\epsilon = \epsilon(\mathbf{k})$  is the energy of the state with wavevector  $\mathbf{k}$ .

The approximation taken is explicitly discussed for each mechanism in turn.

## Six-Band $\mathbf{k} \cdot \mathbf{p}$ Model

As previously described, the valence band is described using a  $6 \times 6$   $\mathbf{k} \cdot \mathbf{p}$  model. This gives a band structure that allows effects of alternative channel and substrate orientations to be properly included.

To maintain computational efficiency, a spherically averaged density-of-states (DOS) mass is used to calculate scattering rates that are tabulated as a function of energy during the initialization phase. This mass is defined as [5]:

$$\frac{m^{3/2}\sqrt{E}}{\sqrt{2\pi^2\hbar^3}} = \frac{1}{(2\pi)^3} \int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta k^2 \left| \frac{\partial E}{\partial k} \right|^{-1} \quad (179)$$

For valence band scattering, the overlap integral is approximated using the expressions given by Wiley [6]. Therefore, for intraband transitions involving the top two bands, the overlap integral is:

$$I(\mathbf{k}, \mathbf{k}') = \frac{1}{4}(1 + 3\cos^2\theta) \quad (180)$$

where  $\theta$  is the angle between the initial and final  $\mathbf{k}$ -vectors. For interband transitions, it is:

$$I(\mathbf{k}, \mathbf{k}') = \frac{3}{4}(\sin^2\theta) \quad (181)$$

For all events involving the spin split-off band, the integral is unity.

---

## Conservation of Energy Momentum

This section discusses conservation of energy momentum.

## Chapter 12: Scattering Models

### Phonon Scattering Models

## Analytic Valley Model

Given a spherical nonparabolic valley model with the following dispersion relation:

$$\varepsilon(k)(1 + \alpha\varepsilon(k)) = \frac{\hbar^2 k^2}{2m^*} \quad (182)$$

the energy-conserving delta function and the momentum-conserving Kroneker delta can be combined into a single energy- and momentum-conserving delta function following [1]:

$$\delta[\varepsilon(k') - \varepsilon(k) \mp \hbar\omega(q)]\delta_{k', k \pm q} = \delta\left[q^2 \pm 2kq\cos\theta \mp \frac{2m^*\omega(q)}{\hbar}\left(1 + 2\alpha\varepsilon(k) \pm \frac{1}{2}\hbar\omega(q)\right)\right] \quad (183)$$

Here, the nonparabolicity of the valley model is included.

## Six-Band $\mathbf{k} \cdot \mathbf{p}$ Model

For the six-band  $\mathbf{k} \cdot \mathbf{p}$  case, the situation is complicated by the use of an effective mass that depends on both energy and the initial and final bands. The energy- and momentum-conserving delta function is treated using a numeric routine for tabulated band-structures.

## Full Band Model

The energy- and momentum-conserving delta function is treated using a numeric routine for tabulated band-structures.

---

## Phonon Scattering Models

For phonon scattering, the transition rate is described by the following general expression [2]:

$$S(k, k') = \frac{\pi|D(q)|^2}{\rho\Omega\omega(q)} \begin{bmatrix} N_q \\ N_q + 1 \end{bmatrix} I(k, k') \delta[\varepsilon(k') - \varepsilon(k) \mp \hbar\omega(q)] \delta_{k', k \pm q} \quad (184)$$

where:

- $D(q)$  defines the coupling strength for scattering between states  $k$  and  $k'$  for the specific phonon mechanism.
- $N_q$  is the phonon occupation number.
- $N_q$  and  $N_q + 1$  denote absorption and emission processes, respectively.

Phonon scattering rates can then be determined by specifying a form for  $D(q)$ , as well as for  $I(k, k')$  and  $N_q$ , then summing over all energy momentum-conserving final states.

## Chapter 12: Scattering Models

### Phonon Scattering Models

In general, the phonon occupation number is given by the Bose–Einstein distribution:

$$N_q = \frac{1}{\exp\left(\frac{\hbar\omega(q)}{k_B T}\right) - 1} \quad (185)$$

---

## Elastic Acoustic Phonon Scattering Model

This model treats acoustic phonon scattering within the elastic approximation and considering a single phonon branch. Since no energy is transferred, the energy- and momentum-conserving delta function (Equation 183) reduces to:

$$\delta[\varepsilon(k') - \varepsilon(k) \mp \hbar\omega(q)]\delta_{k,k' \pm q} = \delta[q^2 \pm 2kq\cos\theta] \quad (186)$$

The phonon occupation is approximated by the equipartition expression [2]:

$$N_q = \frac{k_B T}{\hbar\omega(q)} - \frac{1}{2} \quad (187)$$

where the phonon dispersion relation is here approximated as an isotropic linear function given by:

$$\omega(q) = \frac{1}{3}(u_l + 2u_t)|q| = \bar{u}|q| \quad (188)$$

Here,  $u_l$  and  $u_t$  are the longitudinal and transverse sound velocities of the semiconductor material. The overlap integral  $I(k, k')$  is here taken to be unity.

The phonon coupling is approximated by a scalar-averaged acoustic deformation potential  $D_{ac}$  as [1][2]:

$$D(q) = |q|D_{ac} \quad (189)$$

## Scattering Rate

Given the above approximations and combining equivalent absorption and emission processes, the transition rate is defined that leads to the following scattering rate:

$$\Gamma(k) = \frac{k_B T D_{ac}^2}{4\pi^2 \hbar^2 \rho \bar{u}^2} \int \delta[q^2 \pm 2kq\cos\theta] d^3 k' \quad (190)$$

## Analytic Band Model

From Equation 190, the scattering rate is determined as:

$$\Gamma(k) = \frac{k_B T D_{ac}^2}{2\pi \hbar^2 \rho \bar{u}^2} \int_0^\infty q^2 dq \int_{-1}^1 \delta[q^2 \pm 2kq\cos\theta] d(\cos\theta) \quad (191)$$

## Chapter 12: Scattering Models

### Phonon Scattering Models

Equation 191 is evaluated analytically, resulting in the final rate for intravalley transition of electrons in the  $i^{\text{th}}$  valley as:

$$\Gamma(\varepsilon) = \frac{\sqrt{2}m_i^{*3/2}k_B TD_{\text{ac}}^2}{\pi\hbar^4\rho\pi^2} \sqrt{\varepsilon(1 + \alpha_i\varepsilon)}(1 + 2\alpha_i\varepsilon) \quad (192)$$

where  $m_i^*$  is the DOS effective mass within the  $i^{\text{th}}$  valley.

## Six-Band $\mathbf{k}\cdot\mathbf{p}$ Model

The approach for the six-band  $\mathbf{k}\cdot\mathbf{p}$  model follows that of the analytic band model, but with the following exceptions:

- The overlap integral is non-unity for transitions excluding the SSO band.
- The effective mass is not constant and varies with energy.

The scattering rate is given by:

$$\Gamma(k) = \frac{k_B TD_{\text{ac}}^2}{2\pi\rho\hbar^2n^2} I(k, k') k'^2 \left| \frac{\partial k'}{\partial \varepsilon(k')} \right| \quad (193)$$

For the tabulation of the scattering rates, the following substitution is used, using an energy-dependent DOS mass:

$$k'^2 \left| \frac{\partial k'}{\partial \varepsilon(k')} \right| = \frac{\sqrt{2\varepsilon m^*}^3}{\hbar^3} \quad (194)$$

## Full Band Model

For the full band model, the overlap integral is assumed to be one and the DOS is calculated numerically. The scattering rate is given by:

$$\Gamma(k) = \frac{k_B TD_{\text{ac}}^2}{\rho\hbar^2n^2} g(\varepsilon(k)) \quad (195)$$

where  $g(\varepsilon(k))$  is the DOS.

---

## Inelastic Acoustic Phonon Scattering Model

Inelastic acoustic phonon scattering is treated assuming a single acoustic phonon branch. Like the elastic acoustic phonon scattering model, phonon coupling is approximated by an isotropic deformation potential as [2]:

$$D(\mathbf{q}) = |\mathbf{q}| D_{\text{ac}} \quad (196)$$

## Chapter 12: Scattering Models

### Phonon Scattering Models

A quadratic function is used to approximate the single isotropic phonon branch, following [7], as:

$$\omega(\mathbf{q}) = \omega_0 + \bar{a}|\mathbf{q}| + c|\mathbf{q}|^2 \quad (197)$$

and Equation 185 is used to calculate the phonon occupation  $N_q$  directly. The overlap integral  $I(\mathbf{k}, \mathbf{k}')$  is here taken to be unity.

## Scattering Rate

The scattering rate for inelastic acoustic phonon scattering is approximated as:

$$\Gamma(k) = \frac{D_{ac}^2}{8\pi^2 \rho_k^2} \int \frac{q^2}{\omega(q)} \left[ \begin{array}{c} N_q \\ N_q + 1 \end{array} \right] \delta[\varepsilon(\mathbf{k}') - \varepsilon(\mathbf{k}) \mp \hbar\omega(\mathbf{q})] \delta_{\mathbf{k}', \mathbf{k} \pm \mathbf{q}} d^3 k' \quad (198)$$

## Analytic Band Model

The inelastic acoustic phonon scattering rate is determined from Equation 198, having transformed integration over the final state  $\mathbf{k}'$  to integration over the phonon wavevector  $q$  in polar coordinates as in Equation 177, as:

$$\Gamma(k) = \frac{m^* D_{ac}^2}{4\pi \rho \hbar^2 k} \int_{q_{min}}^{q_{max}} \left[ \begin{array}{c} N_q \\ N_q + 1 \end{array} \right] \frac{q^3}{\omega(q)} dq \quad (199)$$

Evaluation of Equation 199 is performed numerically given the limits of the allowed phonon wavevectors  $q_{min}$  and  $q_{max}$ , which are given by the maximum and minimum  $q$  that satisfies the inequality:

$$-2k \leq \mp q \left( 1 - 2\alpha m^* \left( \frac{\omega(q)}{q} \right)^2 \right) + \frac{2m^* \omega(q)}{\hbar q} (1 + 2\alpha \varepsilon(k)) \leq 2k \quad (200)$$

The phonon wavevector limits  $q_{min}$  and  $q_{max}$  are similarly solved numerically, given the phonon dispersion  $\omega(q)$ .

## Six-Band $\mathbf{k} \cdot \mathbf{p}$ Model

The approach for the six-band  $\mathbf{k} \cdot \mathbf{p}$  model follows that of the analytic band model, but with the following exceptions:

- The overlap integral is non-unity for transitions excluding the SSO band.
- The effective mass is not constant and varies with energy.

The scattering rate is defined as:

$$\Gamma(\varepsilon) = \frac{D_{ac}^2}{4\pi \rho} \int_{q_{min}}^{q_{max}} \left[ \begin{array}{c} N_q \\ N_q + 1 \end{array} \right] \frac{q^2}{\omega(q) k k'} I(\mathbf{k}, \mathbf{k}') |\mathbf{k'}|^2 \left| \frac{\partial \mathbf{k}'}{\partial \varepsilon(\mathbf{k}')} \right| dq \quad (201)$$

## Chapter 12: Scattering Models

### Phonon Scattering Models

For the tabulation of the rates, the following substitution is used, using the energy-dependent DOS mass:

$$k^2 \left| \frac{\partial k'}{\partial \epsilon(k')} \right| = \frac{\sqrt{2\epsilon m^*}^3}{\hbar^3} \quad (202)$$

The limits of integration  $q_{\min}$  and  $q_{\max}$  are given using a numerical root-finding routine with the left-hand side of [Equation 183](#).

## Full Band Model

Inelastic acoustic phonon scattering is not available with full band-structures.

---

## Optical Phonon Scattering Model

Optical phonon coupling is approximated by an isotropic deformation potential, independent of the phonon wavevector, as [\[2\]](#):

$$D(q) = D_{\text{op}} \quad (203)$$

The phonon dispersion is approximated as a constant because the range of phonon wavevectors involved in intervalley transition is small, and the actual optical phonon dispersion does not vary rapidly.

$$\omega(q) = \omega_{\text{op}} \quad (204)$$

As with inelastic acoustic phonon scattering, the phonon occupation  $N_{\text{op}}$ , a constant since the optical phonon energy  $\hbar\omega_{\text{op}}$  is constant, is determined directly following [Equation 185](#). The overlap integral  $I(k, k')$  is here included indirectly.

Following a similar argument to the constant optical phonon dispersion, the overlap integral is assumed constant due to the limited range of phonon wavevectors involved in intervalley transitions. This constant value is then incorporated into the deformation potential as an empirical fitting parameter.

Multiple optical phonon mechanisms can be defined within a material. For each, a value of the optical deformation potential  $D_{\text{op}}$  and the phonon frequency  $\omega_{\text{op}}$  is uniquely specified.

## Scattering Rate

The scattering rate for optical phonon scattering is approximated as:

$$\Gamma(k) = \frac{D_{\text{op}}^2}{8\pi^2 \rho \omega_{\text{op}}} \left[ \frac{N_{\text{op}}}{N_{\text{op}} + 1} \right] \int_{k'} \delta[\epsilon(k') - \epsilon(k) \mp \hbar\omega_{\text{op}}] \delta_{k', k \pm q} d^3 k' \quad (205)$$

## Chapter 12: Scattering Models

### Phonon Scattering Models

## Analytic Band Model

The intervalley optical phonon scattering rate is determined analytically from [Equation 205](#), yielding the final rate:

$$\Gamma(\varepsilon) = \frac{m_f^{*3/2} D_{\text{op}}^2}{\sqrt{2}\pi\hbar^3\omega_{\text{op}}} \left[ \frac{N_{\text{op}}}{N_{\text{op}} + 1} \right] \sqrt{\varepsilon'(1 + \alpha_f\varepsilon')(1 + 2\alpha_f\varepsilon')} \quad (206)$$

where:

- $\varepsilon' = \varepsilon(\mathbf{k}) \pm \hbar\omega_{\text{op}}$  is the final energy after absorption or emission of an optical phonon.
- $m_f^*$  and  $\alpha_f$  are the DOS effective mass and the nonparabolicity factor, respectively, associated with the final valley into which the carrier is scattered.

## Six-Band $\mathbf{k} \cdot \mathbf{p}$ Model

For the six-band  $\mathbf{k} \cdot \mathbf{p}$  model, the optical phonon scattering rate can be found without numeric integration. Again, the main differences to the analytic band model are the energy-dependent effective mass and overlap integral.

For transitions involving only the heavy-hole and light-hole bands, the scattering rate is defined as [\[2\]](#):

$$\Gamma(\varepsilon) = \frac{m_f^{*3/2} D_{\text{op}}^2}{2^{3/2}\pi\hbar^3\omega_{\text{op}}} \left[ \frac{N_{\text{op}}}{N_{\text{op}} + 1} \right] \sqrt{\varepsilon'} \quad (207)$$

where:

- $\varepsilon' = \varepsilon(\mathbf{k}) \pm \hbar\omega_{\text{op}}$  is the final energy after absorption or emission of an optical phonon.
- $m_f^*$  is the DOS mass for the final energy in the final band.

When the spin split-off band is involved, due to the unity overlap integral, the rate becomes:

$$\Gamma(\varepsilon) = \frac{m_f^{*3/2} D_{\text{op}}^2}{\sqrt{2}\pi\hbar^3\omega_{\text{op}}} \left[ \frac{N_{\text{op}}}{N_{\text{op}} + 1} \right] \sqrt{\varepsilon'} \quad (208)$$

## Full Band Model

For the full band model, the scattering rate is defined as:

$$\Gamma(\varepsilon) = \frac{\pi D_{\text{op}}^2}{2\rho\omega_{\text{op}}} \left[ \frac{N_{\text{op}}}{N_{\text{op}} + 1} \right] g(\varepsilon') \quad (209)$$

where  $g(\varepsilon')$  is the density of final states, and an overlap integral of one is assumed.

## Chapter 12: Scattering Models

### Phonon Scattering Models

## Polar-Optical Phonon Scattering Model

The phonon dispersion is approximated as a constant since the range of phonon wavevectors involved in the intervalley transition is small, and the actual optical phonon dispersion does not vary rapidly, as follows:

$$\omega(\mathbf{q}) = \omega_{\text{op}} \quad (210)$$

The squared modulus of the matrix element for polar-optical phonon scattering is given as [4]:

$$|D(\mathbf{q})|^2 = \frac{2e^2 \hbar \omega_{\text{op}}}{q^2} \left( \frac{1}{\kappa_\infty} - \frac{1}{\kappa_0} \right) \quad (211)$$

The overlap is here included and approximated as [2]:

$$I(\mathbf{k}, \mathbf{k}') = \frac{[(1 + \alpha\epsilon)^{1/2}(1 + \alpha\epsilon')^{1/2} + \alpha(\epsilon\epsilon')^{1/2}\cos\theta]^2}{(1 + 2\alpha\epsilon)(1 + 2\alpha\epsilon')} \quad (212)$$

where  $\epsilon' = \epsilon \pm \hbar\omega_{\text{op}}$  is the carrier energy after absorption or emission of an optical phonon.

The carrier–phonon interaction is treated as unscreened in this model.

## Scattering Rate

Given the above approximations and combining equivalent absorption and emission processes, the transition rate is defined, which leads to the following scattering rate:

$$\Gamma(k) = e^2 \omega_{\text{op}} \left( \frac{1}{\kappa_\infty} - \frac{1}{\kappa_0} \right) \int_0^\pi \sin\theta d\theta \int_0^\infty \frac{I(\mathbf{k}, \mathbf{k}')}{q^2} \begin{bmatrix} N_{\text{op}} \\ N_{\text{op}} + 1 \end{bmatrix} \delta[\epsilon(\mathbf{k}') - \epsilon(\mathbf{k}) \mp \hbar\omega_{\text{op}}] \delta_{\mathbf{k}', \mathbf{k} \pm \mathbf{q}} dq \quad (213)$$

## Analytic Band Model

The total scattering rate is evaluated analytically as [2]:

$$\Gamma(\epsilon) = \frac{e^2 \sqrt{m} \omega_{\text{op}}}{\sqrt{2}\hbar} \left( \frac{1}{\kappa_\infty} - \frac{1}{\kappa_0} \right) \frac{1 + 2\alpha\epsilon'}{\sqrt{\epsilon(1 + \alpha\epsilon)}} F_0(\epsilon, \epsilon') \begin{bmatrix} N_{\text{op}} \\ N_{\text{op}} + 1 \end{bmatrix} \quad (214)$$

where:

$$F_0(\epsilon, \epsilon') = C^{-1} \left\{ A \ln \left| \frac{\gamma^{1/2}(\epsilon) + \gamma^{1/2}(\epsilon')}{\gamma^{1/2}(\epsilon) - \gamma^{1/2}(\epsilon')} \right| + B \right\} \quad (215)$$

$$A = \{2(1 + 2\alpha\epsilon)(1 + \alpha\epsilon') + \alpha[\gamma(\epsilon) + \gamma(\epsilon')]\}^2 \quad (216)$$

$$B = -2\alpha\gamma^{1/2}(\epsilon)\gamma^{1/2}(\epsilon')\{4(1 + \alpha\epsilon)(1 + \alpha\epsilon') + \alpha[\gamma(\epsilon) + \gamma(\epsilon')]\} \quad (217)$$

$$C = 4(1 + \alpha\epsilon)(1 + \alpha\epsilon')(1 + 2\alpha\epsilon)(1 + 2\alpha\epsilon') \quad (218)$$

## Chapter 12: Scattering Models

### Ionized Impurity Scattering Models

$$N_{\text{op}} = \frac{1}{\exp\left(\frac{\hbar\omega_{\text{op}}}{k_B T}\right) - 1} \quad (219)$$

### Six-Band $\mathbf{k} \cdot \mathbf{p}$ Model

This model is not defined for hole transport.

### Full Band Model

Integration over the energy-conserving final states is performed directly given the band structure, with each transition weighted by the difference between initial and final  $k$ -vectors  $q^2 = |\mathbf{k}' - \mathbf{k}|^2$ .

The dependence of the scattering rate on the initial state  $\mathbf{k}$  means that the tabulation of the scattering rate as a function of energy  $E$  is not straightforward. Two choices are provided: either the average rate over all initial states  $\mathbf{k}$  with energy satisfying  $\epsilon(\mathbf{k}) = E$  is tabulated and applied, or the maximum rate over the same states is tabulated and used together with a rejection calculated for each event and its specific initial  $k$ -vector.

The `rate` parameter of the mechanism controls the choice; it can be set to either `average` or `maximum`. The default is to tabulate the maximum and use a rejection, which is the most accurate but also the most computationally expensive.

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## Ionized Impurity Scattering Models

This section discusses the ionized impurity scattering models.

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### Brooks–Herring Model

The scattering potential for this model of ionized impurity scattering is given by the screened Coulomb potential [8]:

$$U(r) = \frac{Ze^2}{\kappa r} \exp(-\beta r) \quad (220)$$

Here,  $\beta$  is the inverse screening length and is determined given the electron carrier concentration  $n$  locally on the mesh, given the following form [9][10]:

$$\beta^2 = \frac{4\pi e^2}{\kappa k_B T} \frac{\partial n}{\partial \eta_n} \quad (221)$$

where  $\eta_n$  is the Fermi level associated with the electron carrier concentration  $n$ .

## Chapter 12: Scattering Models

### Ionized Impurity Scattering Models

$\frac{\partial n}{\partial \eta_n}$  is determined directly from the Fermi integrals  $F_{1/2}(\eta)$  and  $F_{-1/2}(\eta)$  using [9]:

$$\frac{\partial n}{\partial \eta_n}(n, N_C) = N_C \left[ F_{-1/2}(\eta) + \frac{15\alpha k_B T}{4} F_{1/2}(\eta) \right] \quad (222)$$

The second term in brackets is a first-order correction to account for the valley nonparabolicity, and  $N_C$  is the effective conduction band DOS (see Part III).

## Dynamic Screening

As an alternative to the dynamic static screening model previously described, a model for dynamic screening of ionized impurities by mobile carriers is available that uses the Lindhard dielectric function.

The Lindhard dielectric function for the limit of zero frequency (the potential is considered time independent) is given by:

$$\epsilon(q, 0) = \frac{\beta^2}{q^2} G(q, \eta) \quad (223)$$

where the screening function  $G$  is given by (assuming an overlap integral of unity here):

$$G(\xi, \eta) = \frac{1}{F_{-1/2}(\eta) \xi \sqrt{\pi}} \int_0^\infty \frac{x}{1 + \exp(x^2 - \eta)} \ln \left| \frac{x + \xi}{x - \xi} \right| dx \quad (224)$$

$$\text{where } \xi^2 = \frac{\hbar^2 q^2}{8m^* k_B T} \text{ and } x^2 = \frac{\hbar^2 k^2}{2m^* k_B T}.$$

A similar function is applied for both electron and hole scattering with only minor differences to account for the band structure and the overlap integral.

This function is precalculated and tabulated at initialization for efficiency. Dynamic screening is not available with full band models.

## Scattering Rate

Given the above, the scattering rate is given by:

$$\Gamma(k) = \frac{8\pi Z^2 e^4 N_i}{\hbar \kappa^2} \int_0^\pi \sin \theta d\theta \int_0^\infty \frac{k'^2}{\beta^2 + q^2} \delta[\epsilon(k') - \epsilon(k)] \delta_{k', k \pm q} dk' \quad (225)$$

## Analytic Band Model

Equation 225 is solved analytically for the spherical nonparabolic valley model, obtaining:

$$\Gamma(k, \beta) = \frac{2^{9/2} m^{*3/2} \pi Z^2 e^4 N_i}{\kappa^2 \hbar^4 \beta^2} \frac{\sqrt{\varepsilon(k)(1 + \alpha\varepsilon(k))}(1 + 2\alpha\varepsilon(k))}{(1 + 4k^2/\beta^2)} \quad (226)$$

This rate is a function of the screening (determined locally). So, an initial rate is tabulated based on the maximum-expected rate given the initial solution within the simulation domain. If a particle free flight is terminated with the selection of this mechanism, then a rejection technique is used, having calculated the local rate to accept or reject the event as a real scattering event. If the local rate exceeds the tabulated rate, then the event is accepted and the tabulated rate is amended accordingly.

## Six-Band $\mathbf{k} \cdot \mathbf{p}$ Model

Due to the inclusion of the non-unity overlap integral and in order to preserve generality among the valence bands, a numeric integration is used for the scattering rate:

$$\Gamma(k, \beta) = \frac{2^{7/2} m^{*3/2} \pi Z^2 e^4 N_i}{\kappa^2 \hbar^4} \sqrt{\varepsilon(k)} \int_0^\pi \frac{I(\mathbf{k}, \mathbf{k}') \sin \theta}{(2k^2(1 - \cos \theta) + \beta^2)^2} d\theta \quad (227)$$

## Full Band Model

For the full band model, the scattering rate is given by:

$$\Gamma_k = \frac{N_i Z^2 e^4}{4\pi^2 \hbar \kappa^2} \int_{\mathbf{k}'} \frac{1}{(q^2 + \beta^2)^2} \delta(\varepsilon(k') - \varepsilon(k)) d^3 k' \quad (228)$$

Here, the integral is evaluated using a DOS term that accounts for the  $q$ -vector and inverse screening length.

## Ridley's Third-Body Exclusion Model

The Ridley model of ionized impurity scattering [11] follows the Brooks–Herring model. It differs in that, while for the Brooks–Herring model the interaction between a carrier and an ion is considered in isolation and defined for arbitrary separations, the interaction within Ridley's model is limited in range by the proximity of neighboring impurity ions.

The average separation of impurity ions is approximated as [12]:

$$a = (2\pi N_i)^{-1/3} \quad (229)$$

## Scattering Rate

The scattering rate is defined in terms of the Brooks–Herring rate  $\Gamma_{\text{BH}}(k)$ , previously described, and the average inter-ion separation  $a$  as [13]:

$$\Gamma(k) = \frac{\nabla_k \varepsilon(k)}{\hbar a} \left[ 1 - \exp\left(\frac{\nabla_k \varepsilon(k)}{\hbar a \Gamma_{\text{BH}}(k)}\right) \right] \quad (230)$$

where  $\frac{1}{\hbar} \nabla_k \varepsilon(k)$  is the band-dependent carrier velocity.

## Analytic Band Model

Given the analytic valley model (see [Analytic Valley Model on page 356](#)), the energy and the carrier velocity are given as:

$$\begin{aligned} \varepsilon(k)(1 + \alpha \varepsilon(k)) &= \frac{\hbar^2 k^2}{2m^*} \\ \frac{1}{\hbar} \nabla_k \varepsilon(k) &= \frac{\hbar k}{m^*(1 + 2\alpha \varepsilon(k))} \end{aligned} \quad (231)$$

which, together with the Brooks–Herring rate  $\Gamma_{\text{BH}}(k)$ , completely defines the scattering rate.

The Ridley third-body screening rate depends on the local total impurity concentration and the carrier density through the Brooks–Herring rate  $\Gamma_{\text{BH}}(k)$ . Like Brooks–Herring scattering, a maximum rate is tabulated at the start of the simulation and individual scattering events are thereafter accepted or rejected based on the local scattering rate, which is determined using local impurity and carrier concentrations. Again, as with the Brooks–Herring model of impurity scattering, if the local rate exceeds the tabulated rate, then the scattering rate table is updated.

## Six-Band $k \cdot p$ Model

The same approach is used for the six-band  $k \cdot p$  case, with the energy-dependent effective mass used to calculate  $\nabla_k \varepsilon(k)$ .

## Full Band Model

For the full band model, the scattering rate as defined by [Equation 230](#) is used along with the full band model for the Brooks–Herring rate.

## Alloy Scattering Model

Alloy scattering is based on a model originally developed by Mott [14] that assumes a model based on a “square-well” potential,  $\Delta U$ , given as:

$$\Delta U = \begin{cases} E_0 - E'_0 & r \leq r_0 \\ 0 & r > r_0 \end{cases} \quad (232)$$

where  $r_0$  is the radius of the Wigner–Seitz cell and  $E_0$  is the energy of the band edge. This is used to represent the different potentials of the two atom species experienced by an electron as it travels through the lattice. The choice of  $r_0$  is arbitrary, but an approach based on the nearest-neighbor separation is assumed to be realistic [15]:

$$r_0 = \frac{\sqrt{3}}{4}a_0 \quad (233)$$

where  $a_0$  is the lattice parameter.

Using this “square-well” potential, Harrison and Hauser defined a scattering matrix element as [15]:

$$|M(k, k')|^2 = \frac{3}{16}\pi^2 x(1-x) \frac{N}{N} (\Delta E)^2 \quad (234)$$


---

## Analytic Band Model

Equation 235 is solved analytically for the nonparabolic valley model, obtaining [16]:

$$\Gamma(k) = \frac{3\pi m^{*3/2}}{32\sqrt{2}\hbar^4} a_0^3 x(1-x) D_{al}^2 d \sqrt{E(1+\alpha E)} (1+2\alpha E) \quad (235)$$

where:

- $m^*$  is the DOS effective mass.
- $a_0$  is the lattice constant.
- $x$  is the alloy fraction of the second minor material.
- $d$  is the degree of disorder parameter (where 0 signifies perfect order and 1 signifies maximum disorder).
- The alloy scattering potential,  $D_{al}$ , can be taken as a difference in electron affinities, or as an electronegative difference, and is often used to fit to experimental data.

## Six-Band $k \cdot p$ Model

Again, the main differences to the analytic band model are the energy-dependent effective mass and the overlap integral. The scattering rate is then given as:

$$\Gamma(k) = \frac{m^{3/2}}{2^{5/2} \pi \hbar^3} a_0^3 x(1-x) D_{\text{al}}^2 d\sqrt{E} \int_{-1}^1 I(\mathbf{k}, \mathbf{k}') d(\cos \theta) \quad (236)$$


---

## Full Band Model

For the full band model, the matrix element given in [Equation 235](#) is used, giving a scattering rate of the form:

$$\Gamma(k) = \frac{\pi D_{\text{al}}^2 x(1-x) V}{\hbar} g(\varepsilon(k)) \quad (237)$$

where  $g(\varepsilon(k))$  is the density of final states and an overlap integral of unity is assumed.

---

## Surface Roughness Scattering Model

The squared modulus of the matrix element for surface roughness scattering is given as [\[17\]](#):

$$|M(q)|^2 = e^2 E_{\text{eff}}^2 |\Delta(q_{\parallel})|^2 I(\mathbf{k}, \mathbf{k}') \quad (238)$$

where  $e$  is the electronic charge,  $E_{\text{eff}}$  is the effective field, and  $\Delta(q_{\parallel})$  is the autocorrelation function given as a function of the momentum transfer parallel to the interface  $q_{\parallel}$ .

An exponential autocorrelation function is assumed for both electron and hole scattering [\[18\]](#):

$$|\Delta(q_{\parallel})|^2 = \frac{\pi \Delta_{\text{RMS}}^2 L^2}{\left(1 + \frac{1}{2} L^2 |q_{\parallel}|^2\right)^{3/2}} \quad (239)$$

Here,  $\Delta_{\text{RMS}}$  and  $L_c$  are the RMS height and the correlation length describing the surface. Common values are used for both electron and hole scattering.

Scattering is treated elastically and in the plane of the rough surface. The final state is defined by the scattering angle  $\phi$  between the initial and final  $\mathbf{k}$ -vectors, such that the momentum transfer is given as:

$$|q_{\parallel}|^2 = 2|k_{\parallel}|^2(1 - \cos \phi) \quad (240)$$

where  $k_{\parallel}$  is the projection of the wavevector onto the surface.

## Scattering Rate

The scattering rate can be determined from the matrix element and the autocorrelation function as:

$$\Gamma(k) = \frac{e^2 E_{\text{eff}}^2 \Delta_{\text{RMS}}^2 L^2}{2\hbar} \int_0^{2\pi} d\phi \int_0^\infty \frac{k'_{\parallel} \delta[\varepsilon(k_{\parallel}) - \varepsilon(k'_{\parallel})]}{(1 + L^2 k_{\parallel}^2 (1 - \cos\phi))^{3/2}} I(k, k') dk'_{\parallel} \quad (241)$$

The integration over the final states is restricted to the 2D plane parallel to the surface, and this integration is performed for the  $i$  bands in which an energy-conserving state exists with final perpendicular momentum:

$$k'_{\perp} = k_{\perp} + \mathbf{F} dt \cdot \hat{\mathbf{n}} \quad (242)$$

where  $\hat{\mathbf{n}}$  is the unit vector normal to the rough interface. The number of energy-conserving states with varying perpendicular momentum depends on the band structure and orientation.

---

## Analytic Band Model

The overlap integral  $I(k, k')$  is here taken to be unity, and the scattering rate defined as:

$$\Gamma(k) = \frac{e^2 E_{\text{eff}}^2 \Delta_{\text{RMS}}^2 L^2 m^*(1 + 2\alpha\varepsilon(k))}{2\hbar^3} \sum_i \int_0^{2\pi} d\phi \int_0^\infty \frac{k'_{\parallel} \delta[\varepsilon(k_{\parallel}) - \varepsilon(k'_{\parallel})]}{(1 + L^2 k_{\parallel}^2 (1 - \cos\phi))^{3/2}} dk'_{\parallel} \quad (243)$$

The maximum scattering rate, defined when  $k_{\parallel} = 0$ , is calculated for each rough interface. This maximum is based on the maximum confining field,  $E_{\max}$ , and the number of perpendicular momentum-conserving states,  $N$ , at each interface:

$$\Gamma_{\max} = N \frac{\pi m^* e^2 E_{\max}^2 \Delta_{\text{RMS}}^2 L^2}{\hbar^3} \quad (244)$$

The maximum rate over all interfaces is tabulated for determination of free-flight times and scattering event selection.

Upon selection of a surface roughness scattering event, a rejection technique is implemented based on the local confining field normal to the interface and the number of perpendicular momentum-conserving states to account for the local scattering rate. By using a local field for the rejection, a position dependency is defined.

In the case of multiple rough surfaces with the same normal and with overlapping projections along this normal, scattering from one surface is defined only if the particle undergoing scattering is closer to the intended surface than any other. This is due to the rejection technique being based on a local field, which is implicitly expected to decrease with distance from the interface but which might increase under the influence of other interfaces.

## Six-Band $k \cdot p$ Model

For the six-band  $k \cdot p$  approach, the 2D DOS mass  $m_{\parallel}^*$  is used and is defined similarly to the 3D version given in [Equation 179 on page 357](#):

$$m_{\parallel}^* = \frac{\hbar^2}{2\pi} \int_0^{2\pi} d\phi k \left| \frac{\partial E}{\partial k} \right|^{-1} \quad (245)$$

The scattering rate is then given as:

$$\Gamma(k) = \frac{e^2 E_{\text{eff}}^2 \Delta_{\text{RMS}}^2 L^2}{2\pi\hbar} \int_0^{2\pi} \frac{I(k, k')}{(1 + L^2 k_{\parallel}^2 (1 - \cos\phi))^{3/2}} k' \left| \frac{\partial E}{\partial k} \right| d\phi \quad (246)$$

This gives a final scattering rate defined as:

$$\Gamma(k) = \frac{m_{\parallel}^* e^2 E_{\text{eff}}^2 \Delta_{\text{RMS}}^2 L^2}{2\pi\hbar} \int_0^{2\pi} \frac{I(k, k')}{(1 + L^2 k_{\parallel}^2 (1 - \cos\phi))^{3/2}} d\phi \quad (247)$$


---

## Full Band Model

For the full band model, the scattering rate is given by:

$$\Gamma(k) = \frac{A}{4\pi^2} \frac{2\pi^2 E_{\text{eff}}^2 \Delta_{\text{RMS}}^2 L^2}{\hbar A} \int \frac{dk'}{\left(1 + \frac{1}{2} L^2 |q^2| \right)^{3/2}} \quad (248)$$

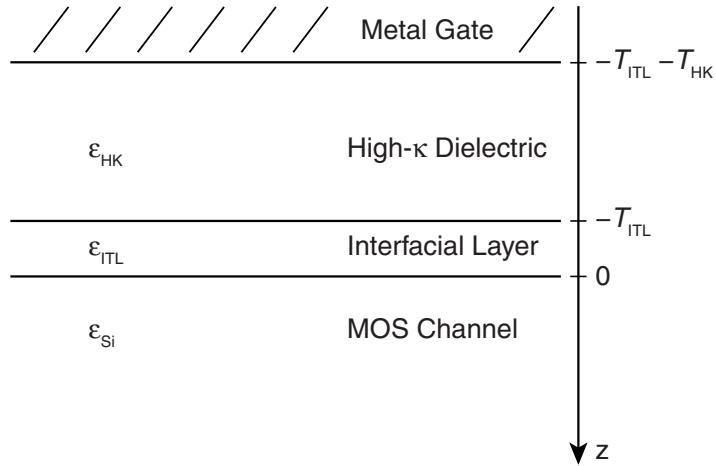
An overlap integral of one is assumed and integration over final states is performed directly. As scattering rates are tabulated over energy, it is the maximum rate over degenerate  $k$ -states that is tabulated and a rejection technique is employed.

---

## Remote Coulomb Scattering Model

This model is based on a general treatment of Coulomb scattering provided by Esseni *et al.* [\[19\]](#), and it assumes a metal–high-k–oxide gate stack as shown in [Figure 39](#). The model is consistent with a multi-subband approach to transport, considering the solutions to the carrier wavefunction consistently with the Poisson equation. Therefore, this model can be applied to 1D transport such as in a nanowire, but it can be used with 2D confinement such as in MOSFETs.

Figure 39 Gate stack model based on Esseni et al., p. 416 [19]



## Perturbation Potential

The perturbation potential is provided by Esseni et al. [19] as the potential solution associated with a single charge located at  $z_0$  within the gate stack (see Figure 39). The potential is given as the Fourier transform of the real-space potential, defined along the z-direction, as:

$$\begin{aligned}\phi_{pc}(q, z, z_0)_{HK} &= \frac{e}{2q\epsilon_0\epsilon_{HK}} e^{-q|z-z_0|} + A_1 e^{qz} + A_2 e^{-qz} \\ \phi_{pc}(q, z, z_0)_{ITL} &= \frac{e}{2q\epsilon_0\epsilon_{ITL}} e^{-q|z-z_0|} + A_3 e^{qz} + A_4 e^{-qz} \\ \phi_{pc}(q, z, z_0)_{Si} &= \frac{e}{2q\epsilon_0\epsilon_{Si}} e^{-q|z-z_0|} + A_5 e^{-qz}\end{aligned}\quad (249)$$

The potential solution within the gate stack, together with the continuity of the potential and the displacement field over the material boundaries, defined a set of five simultaneous equations with five unknown coefficients  $A_1, \dots, A_5$ .

The scattering potential defined within the semiconductor is determined by the coefficient  $A_5(q)$ , which is solved for the given gate stack model.

## Matrix Element

The Esseni model [19] considers a general distribution of trapped charges throughout the gate dielectrics. To simplify the model for computational efficiency, this model considers only trapped charges at material interfaces.

## Chapter 12: Scattering Models

### Remote Coulomb Scattering Model

The scattering matrix associated with this model is given by:

$$|M_{n,n'}(k, k')|^2 = \frac{1}{A_{\text{norm}}} [ |M_{n,n'}^{(0)}(k, k', -T_{\text{ITL}})|^2 N_{\text{HK/ITL}} + |M_{n,n'}^{(0)}(k, k', 0)|^2 N_{\text{Si/ITL}} ] \quad (250)$$

[Equation 250](#) considers scattering from both interfaces and is split into two separate squared matrix elements to be implemented as two separate mechanisms, one for each material interface:

$$|M_{n,n'}(k, k')|_{\text{OX}}^2 = \frac{1}{A_{\text{norm}}} |M_{n,n'}^0(k, k', 0)|^2 N_{\text{Si/ITL}} \quad (251)$$

$$|M_{n,n'}(k, k')|_{\text{HK}}^2 = \frac{1}{A_{\text{norm}}} |M_{n,n'}^0(k, k', -T_{\text{ITL}})|^2 N_{\text{HK/ITL}} \quad (252)$$

## Scattering Rate

Scattering is considered within the plane parallel to the material interface. The scattering rate is defined as the integral of the transition rate over final states as:

$$\Gamma(E(k_{||})) = \frac{1}{2\pi\hbar} \int_0^{2\pi} d\phi \int_0^{\infty} dq |M(k_{||}, k_{||} + q)|^2 \delta[E(k_{||} + q) - E(k_{||})] dq \quad (253)$$

## Analytic Bands

For spherical nonparabolic bands, the scattering rate can be written as:

$$\begin{aligned} \Gamma(E(k_{||})) &= \frac{\alpha}{\pi\hbar} \int_{\phi_{\min}}^{\phi_{\max}} d\phi \int_0^{\infty} dq |M(k_{||}, k_{||} + q)|^2 \delta[\sqrt{1 + 4\alpha\gamma(k_{||}^2 + q^2 + 2k_{||}q\cos(\phi))} - \sqrt{1 + 4\alpha\gamma(k_{||}^2)}] dq \\ &= \frac{2m(1 + 4\alpha\gamma(k))}{\pi\hbar^3} \int_{\pi/2}^{\pi} d\phi |M(k_{||}, k_{||} + q)|^2 \end{aligned} \quad (254)$$

## Six Band $k \cdot p$ Model

For the six band  $k \cdot p$  model, the same approach as for analytic bands is used, making the necessary adjustments for the effective mass and overlap integral.

## Full Band Model

Remote Coulomb scattering is not defined for the full band model.

## Chapter 12: Scattering Models

### Pauli Exclusion Principle

---

## Pauli Exclusion Principle

The Pauli exclusion principle is included using a formulation developed by Uengersboeck and Kosina [20] that is based on a reformulation of the degenerate scattering operator given as:

$$\begin{aligned} Q[f]_k &= \int f_{k'}(1-f_k)S_{k',k}dk' - \int f_k(1-f_{k'})S_{k,k'}dk' \\ &= \int f_{k'}S_{k',k} - f_kS_{k,k'} + f_kf_{k'}(S_{k,k'} - S_{k',k})dk' \end{aligned} \quad (255)$$

This expression can be simplified by using a symmetric approximation with respect to the initial and final states  $k$  and  $k'$ , respectively:

$$f(k)f(k') \approx \frac{1}{2}(f(k)f_{\text{FD}}(k') + f_{\text{FD}}(k)f(k')) \quad (256)$$

where  $f_{\text{FD}} = \left( \exp\left(\frac{E-E_F}{k_B T}\right) + 1 \right)^{-1}$  is the equilibrium Fermi–Dirac distribution.

Using this approximation, the scattering operator can be defined in terms of a modified transition rate and scattering rate:

$$\hat{Q}[f]_k = \int \hat{f}(k')\hat{S}_{k',k}dk' - f(k)\hat{\lambda}_k \quad (257)$$

with:

$$\hat{S}_{k',k} = S_{k,k'}\left(1 - \frac{1}{2}f_{\text{FD}}(k')\right) + S_{k',k}\frac{1}{2}f_{\text{FD}}(k') \quad (258)$$

$$\hat{\lambda}_k = \int \hat{S}_{k',k}dk' \quad (259)$$

The principle of detailed balance can then be used to find  $S_{k',k}$  in terms of  $S_{k,k'}$ . Therefore, a modified scattering rate can be found for a given scattering mechanism.

The Pauli exclusion principle is only considered in the application of inelastic scattering. Modification with this scheme is made to optical phonon absorption and emission such that the modified scattering rates become respectively:

$$\hat{\lambda}_{ab} = \lambda_{ab} \cdot \left(1 + \frac{1}{2} \frac{f_{\text{FD}}(E')}{N_0}\right) \quad (260)$$

$$\hat{\lambda}_{em} = \lambda_{em} \cdot \left(1 - \frac{1}{2} \frac{f_{\text{FD}}(E')}{N_0 + 1}\right) \quad (261)$$

where  $E'$  denotes the final energy, and  $N_0$  is the phonon occupation function.

With increased degeneracy,  $f_{\text{FD}}(E) \rightarrow 1$  and the modified absorption rates increase, while the modified emission rates decrease. Maximum rates are tabulated in both cases and

## Chapter 12: Scattering Models

### References

scattering rates are rejected, dependent on the local level of degeneracy, to reflect the occupation of final states.

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## Chapter 12: Scattering Models

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# 13

## Binary Alloy Semiconductor Material Models

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*This chapter describes the binary alloy semiconductor material models as defined and used in Garand.*

---

### Overview of Binary Alloy Semiconductors

A binary alloy semiconductor is based on interpolated values for each parameter based on the mole fraction, and the defined parameters closely follow those of a typical semiconductor as detailed in [Chapter 8 on page 265](#).

**Note:**

The alloy fraction is related to the materials in the form  $\langle\text{materialA}\rangle_{1-x}$   $\langle\text{materialB}\rangle_x$ . This becomes  $\text{In}_{1-x}\text{Ga}_x\text{As}$  for InGaAs and  $\text{Si}_{1-x}\text{Ge}_x$  for SiGe.

The material description for each alloy material effectively describes the interpolation function for each parameter. You define the value for each parameter in one of the following ways:

- Entirely within the alloy material files using constant and piecewise interpolation options
- Based on the values from the two constituent materials, with the alloy material file defining the interpolation

A binary material must define an alloy fraction and can also define two constituent materials. If these two materials are defined, then the binary material parameter file is used to define the interpolation between each parameter. If these two materials are not defined, then all values must be defined in the alloy material parameter file. Defining only one material returns an error.

To modify the parameters listed in [Table 63](#), the following syntax applies:

```
material <material>.⟨parameter⟩ <value>
```

## Chapter 13: Binary Alloy Semiconductor Material Models

### Binary Scattering Parameters

Table 63 Material bulk model parameters (fixed properties only)

Parameter symbol	Parameter name	Description	Default	Unit
$x$	x_fraction	Binary alloy fraction	Must be defined	–
$A_{1-x}$	material1	Binary alloy constituent material A	Optional	–
$B_x$	material2	Binary alloy constituent material B	Optional	–

---

## Binary Scattering Parameters

The binary scattering mechanism definition extends the existing semiconductor material scattering mechanism definitions (see [Chapter 11 on page 339](#)).

To modify the binary scattering parameters listed in subsequent chapters, use the following syntax:

```
<material>.<bandcontainer>.<band>.<valley>.<mechanism>.<parameter>  
<value>
```

All mechanisms available for standard semiconductors can be used for binary alloy materials.

---

## Alloy Scattering

Alloy scattering is only available for alloy materials.

Table 64 Alloy scattering parameter (fixed properties only)

Parameter symbol	Parameter name	Description	Default	Unit
$U$	U	Alloy potential	0.0	eV

## **Part IV: Default Material Definitions**

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This part of the *Garand User Guide* contains the following chapters:

- [Chapter 14, Default Materials](#)
- [Chapter 15, Silicon Material Model](#)
- [Chapter 16, Germanium Material Model](#)
- [Chapter 17, Indium Gallium Arsenide Material Model](#)
- [Chapter 18, Indium Aluminum Arsenide Material Model](#)
- [Chapter 19, Gallium Arsenide Material Model](#)
- [Chapter 20, Indium Arsenide Material Model](#)
- [Chapter 21, Aluminum Arsenide Material Model](#)
- [Chapter 22, Silicon Germanium Binary Alloy Material Model](#)
- [Chapter 23, Indium Gallium Arsenide Binary Alloy Material Model](#)
- [Chapter 24, Indium Aluminum Arsenide Binary Alloy Material Model](#)
- [Chapter 25, Gallium Nitride Material Model](#)

# 14

## Default Materials

---

*This chapter describes the default materials used in Garand and Garand MC.*

All materials are identified by unique names that allow you to assign nondefault model definitions and parameter values by using the input file (see [Chapter 5 on page 186](#)). These names are immutable.

---

### Default Semiconductor Materials

Garand provides default models for common semiconductor materials (see [Chapter 8 on page 265](#)).

Both InGaAs and InAlAs are provided with default models for fixed fractions. These are chosen to be lattice matched and represent the most technologically common form.

*Table 65 Default semiconductor materials with their status in terms of calibration to experimentally measured bulk data*

Default semiconductor material	Material name	Garand calibrated		Garand MC calibrated	
		Electrons	Holes	Electrons	Holes
Silicon	Silicon	Complete	Complete	Complete	Complete
Germanium	Germanium	Pending	Complete	Pending	Complete
In <sub>0.53</sub> Ga <sub>0.47</sub> As	In53Ga47As_fixed	Complete	Pending	Complete	Pending
In <sub>0.52</sub> Al <sub>0.48</sub> As	In52Al48As_fixed	Complete	Pending	Complete	Pending
GaAs	GaAs	Pending	Pending	Complete	Pending
InAs	InAs	Pending	Pending	Complete	Pending
AlAs	AlAs	Pending	Pending	Complete	Pending

## Chapter 14: Default Materials

### Default Insulator Materials

Table 65 Default semiconductor materials with their status in terms of calibration to experimentally measured bulk data (Continued)

Default semiconductor material	Material name	Garand calibrated		Garand MC calibrated	
		Electrons	Holes	Electrons	Holes
GaN	GaN	Pending	Pending	Complete	Pending
Si <sub>1-x</sub> Ge <sub>x</sub>	SiYGeX	Pending	Pending	Complete	Complete
In <sub>1-x</sub> Ga <sub>x</sub> As	InYGaXAs	Pending	Pending	Complete	Pending
In <sub>1-x</sub> Al <sub>x</sub> As	InYAlXAs	Pending	Pending	Complete	Pending

## Calibrated Material Carriers

Calibration of transport for both electrons and holes in each default material is indicated in Table 65. Complete calibrations are provided for the most relevant material carriers, while calibrations are pending for material carriers that are not as technologically relevant.

## Default Insulator Materials

Garand provides default models for common insulator materials (see [Chapter 9](#) on page 308).

Table 66 Default insulator materials

Default insulator material	Material name
Silicon dioxide (SiO <sub>2</sub> )	Oxide
Silicon oxynitride (SiO <sub>x</sub> N <sub>y</sub> )	Oxynitride
Silicon nitride (Si <sub>3</sub> N <sub>4</sub> )	Nitride
Aluminum oxide (Al <sub>2</sub> O <sub>3</sub> )	Al2O3
Hafnium oxide (HfO <sub>2</sub> )	HfO2
Air	Air   Gas

# 15

## Silicon Material Model

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*This chapter describes the silicon material model.*

---

### Bulk Material Model

This section describes the bulk material model for silicon.

---

#### Parameters of Bulk Material Model

To change the default parameter values in [Table 67](#), use the following input file syntax:

```
MATERIAL silicon.<parameter> <value>
```

*Table 67 Bulk material model parameters*

Parameter symbol	Parameter name	Description	Default	Unit
<b>Crystal lattice and orientation in simulation domain</b>				
a	a	Magnitude of lattice vector a	5.43	Å
b	b	Magnitude of lattice vector b	5.43	Å
c	c	Magnitude of lattice vector c	5.43	Å
$\alpha$	alpha	Angle between b and c	90	degree
$\beta$	beta	Angle between c and a	90	degree
$\gamma$	gamma	Angle between a and b	90	degree
$\langle hkl \rangle_x$	x	Orientation in the x-direction	1 1 0	—

## Chapter 15: Silicon Material Model

### Bulk Material Model

*Table 67 Bulk material model parameters (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$\langle hkl \rangle_z$	z	Orientation in the z-direction	0 0 1	–
<b>Bulk electrical and mechanical properties</b>				
$\kappa$	permittivity	Relative dielectric constant	11.7	–
$\kappa_\infty$	k_inf	High-frequency permittivity	16.0	–
$\rho$	density	Mass density	2.329	g/cm <sup>3</sup>
$C_{11}$	C11	Elastic stiffness matrix element	168.3	GPa
$C_{12}$	C12	Elastic stiffness matrix element	66.8	GPa
$C_{44}$	C44	Elastic stiffness matrix element	79.9	GPa

## Band-to-Band Tunneling Parameters

To change the default parameter values for the Kane model, listed in [Table 68](#), use the following input file syntax:

```
MATERIAL Silicon.BTBT.<parameter> <value>
```

*Table 68 Band-to-band tunneling parameters*

Parameter symbol	Parameter name	Description	Default	Unit
$D_{TA}$	DTA	Acoustic phonon deformation potential	$2.45 \times 10^{10}$	eV
$\epsilon_{TA}$	epsilonTA	Acoustic phonon energy	$19 \times 10^{-3}$	eV

## Chapter 15: Silicon Material Model

### Conduction Band Model

---

## Conduction Band Model

This section describes the conduction band model.

---

### Band Edge Parameters

To change the default parameter values of the conduction band container model, listed in [Table 69](#), use the following input file syntax:

```
MATERIAL Silicon.conduction.<parameter> <value>
```

*Table 69 Parameters of conduction band container model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Conduction band energy with respect to vacuum	4.0727	eV
$m_{dg_x}$	$dgx$	Electron density gradient effective x-mass	0.3	$m_e$
$m_{dg_y}$	$dgy$	Electron density gradient effective y-mass	0.3	$m_e$
$m_{dg_z}$	$dgz$	Electron density gradient effective z-mass	0.3	$m_e$

To change the default parameter values of the conduction bands in the container model, listed in [Table 70](#), use the following input file syntax:

```
MATERIAL Silicon.conduction.<band>.<parameter> <value>
```

*Table 70 Parameters of conduction band model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Conduction band energy with respect to container energy	0.0	eV
$model$	$model$	Model used for transport in this band	ema	—

## Chapter 15: Silicon Material Model

### Conduction Band Model

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## Mobility Models

The conduction band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models.

### Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 71](#), use the following input file syntax:

```
MATERIAL Silicon.conduction.constant.<parameter> <value>
```

*Table 71 Parameters of constant mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	1417.0	$\text{cm}^2/\text{Vs}$
$\zeta$	zeta	Fitting parameter	2.5	—

### Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 72](#), use the following input file syntax:

```
MATERIAL Silicon.conduction.Arora.<parameter> <value>
```

*Table 72 Parameters of Arora mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min}$	mumin	Minimum mobility	88.0	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	1340.0	$\text{cm}^2/\text{Vs}$
$N_0$	n0	Reference concentration	$1.25 \times 10^{17}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.88	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.33	—

## Chapter 15: Silicon Material Model

### Conduction Band Model

*Table 72 Parameters of Arora mobility model (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

## Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 73](#), use the following input file syntax:

```
MATERIAL Silicon.conduction.Masetti.<parameter> <value>
```

*Table 73 Parameters of Masetti mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min 1}$	mumin1	Minimum mobility	52.2	$\text{cm}^2/\text{Vs}$
$\mu_{\min 2}$	mumin2	Minimum mobility	52.2	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	1417.0	$\text{cm}^2/\text{Vs}$
$\mu_1$	mul	Maximum mobility	43.4	$\text{cm}^2/\text{Vs}$
$C_r$	cr	Reference concentration	$9.68 \times 10^{16}$	$\text{cm}^{-3}$
$C_s$	cs	Reference solid solubility concentration	$3.43 \times 10^{20}$	$\text{cm}^{-3}$
$p_c$	pc	Reference concentration	0.0	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.68	—
$\beta$	beta	Fitting parameter	2.0	—
$\zeta$	zeta	Fitting parameter	2.5	—

## Chapter 15: Silicon Material Model

### Conduction Band Model

## Low Field: Philips Unified Mobility Model

To change the default parameter values of the Philips unified mobility model, listed in [Table 74](#), use the following input file syntax:

```
MATERIAL Silicon.conduction.Philips.<parameter> <value>
```

*Table 74 Parameters of Philips unified mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min}$	mumin	Minimum mobility	55.2	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	1417.0	$\text{cm}^2/\text{Vs}$
$\alpha$	alpha	Fitting parameter	0.68	—
$C_D$	CD	Reference concentration for ultrahigh-doped donors	0.21	—
$C_A$	CA	Reference concentration for ultrahigh-doped acceptors	0.5	—
$N_{\text{ref}}$	Nref	Reference concentration	$9.68 \times 10^{16}$	$\text{cm}^{-3}$
$N_{D, \text{ref}}$	NDref	Reference concentration	$4.0 \times 10^{20}$	$\text{cm}^{-3}$
$N_{A, \text{ref}}$	NAref	Reference concentration	$7.2 \times 10^{20}$	$\text{cm}^{-3}$
$N_{c, \text{ref}}$	Ncref	Reference concentration	$1.36 \times 10^{20}$	$\text{cm}^{-3}$
$N_{sc, \text{ref}}$	Nscref	Reference surface concentration	$3.97 \times 10^{13}$	$\text{cm}^{-2}$
$m_e$	me	Normalized electron mass	1.0	—
$m_h$	mh	Normalized hole mass	1.25	—
$f_{BH}$	fbh	Brooks–Herring coefficient	3.828	—
$f_{CW}$	fcw	Conwell–Weisskopf coefficient	2.459	—

## Chapter 15: Silicon Material Model

### Conduction Band Model

## Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 75](#), use the following input file syntax:

```
MATERIAL Silicon.conduction.Yamaguchi.<parameter> <value>
```

*Table 75 Parameters of Yamaguchi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

## Perpendicular Field: Lombardi Mobility Model

To change the default parameter values of the Lombardi mobility model, listed in [Table 76](#), use the following input file syntax:

```
MATERIAL Silicon.conduction.Lombardi.<parameter> <value>
```

*Table 76 Parameters of Lombardi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$A$	a	Fitting parameter	2.0	—
$B$	b	Fitting parameter	$4.75 \times 10^7$	cm/s
$C$	c	Fitting parameter	$5.80 \times 10^2$	$\text{cm}^{5/3} \text{V}^{-2/3} \text{s}^{-1}$
$\alpha$	alpha	Fitting parameter	0.0	$\text{cm}^3$
$\delta$	delta	Fitting parameter	$5.82 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$5.82 \times 10^{30}$	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	1.0	—
$\lambda$	lambda	Fitting parameter	0.125	—
$\nu$	nu	Fitting parameter	1.0	—

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### Conduction Band Model

*Table 76 Parameters of Lombardi mobility model (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$N_0$	n0	Fitting parameter	1.0	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	1.0	$\text{cm}^{-3}$
$l_{\text{crit}}$	lcrit	Critical length	$1 \times 10^{-6}$	cm

## Perpendicular Field: Thin-Layer Mobility Model

To change the default parameter values of the thin-layer mobility model, listed in [Table 77](#), use the following input file syntax:

```
MATERIAL Silicon.conduction.Thin_Layer.<parameter> <value>
```

*Table 77 Parameters of thin-layer mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
A	a	Fitting parameter	2.0	–
$\alpha$	alpha	Fitting parameter	0.0	–
$\beta$	beta	Fitting parameter	4	–
$\gamma$	gamma	Fitting parameter	0.29	–
$\delta$	delta	Fitting parameter	$5.82 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$5.82 \times 10^{30}$	$\text{V}^2/\text{cms}$
v	nu	Fitting parameter	1.0	–
$F_{tf0}$	ftf0	Fitting parameter	6250	V/cm
$l_{\text{crit}}$	lcrit	Critical length	$10 \times 10^{-7}$	cm
$\mu_{\text{ac}01}$	muac01	Fitting parameter	315	$\text{cm}^2/\text{Vs}$
$\mu_{\text{ac}02}$	muac02	Fitting parameter	6.4	$\text{cm}^2/\text{Vs}$

## Chapter 15: Silicon Material Model

### Conduction Band Model

*Table 77 Parameters of thin-layer mobility model (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{sp0}$	musp0	Fitting parameter	$1.145 \times 10^{-8}$	$\text{cm}^2/\text{Vs}$
$\mu_{tf0}$	mutf0	Fitting parameter	0.15	$\text{cm}^2/\text{Vs}$
$m_{z1}$	mz1	First ladder mass	0.916	$m_0$
$m_{z2}$	mz2	Second ladder mass	0.19	$m_0$
$N_1$	n1	Fitting parameter	1.0	$\text{cm}^{-3}$
$p_1$	p1	Fitting parameter	0.55	—
$p_2$	p2	Fitting parameter	400	—
$p_3$	p3	Fitting parameter	1.44	—
$t_{\min}$	tmin	Fitting parameter	2	nm
$t_{sp0}$	tsp0	Fitting parameter	0.1	nm
$W_{f01}$	wf01	Fitting parameter	2.91	nm
$W_{f02}$	wf02	Fitting parameter	8.37	nm
$W_{t01}$	wt01	Fitting parameter	$3 \times 10^{-3}$	nm
$W_{t02}$	wt02	Fitting parameter	$3.5 \times 10^{-4}$	nm

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in [Table 78](#), use the following input file syntax:

```
MATERIAL Silicon.conduction.Caughey.<parameter> <value>
```

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### Conduction Band Model

Table 78 Parameters of Caughey–Thomas mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$1.07 \times 10^7$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	0.87	—
$\beta_0$	beta0	Fitting parameter	1.109	—
$\beta_{\text{exp}}$	bexp	Fitting parameter	0.66	—
$\alpha$	alpha	Fitting parameter	0.0	—

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 79](#). To change the default mobility model, use the following input file syntax:

```
MATERIAL Silicon.conduction.mobility.<model> <value>
```

Table 79 Parameters of default mobility model

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley conduction band model consists of the valley minima listed in [Table 80](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL Silicon.conduction.<band>.<valley> REMOVE
```

## Chapter 15: Silicon Material Model

### Conduction Band Model

Table 80 Names of conduction band minima

Conduction band minimum	Valley name
C1	
X	X1, X2, X3, X4, X5, X6
L	L1, L2, L3, L4, L5, L6, L7, L8
C2	
$\Gamma$	G

## Position and Orientation

Valley minima differ in their position and orientation, the default values of which are shown in [Table 83](#), [Table 84 on page 398](#), and [Table 85 on page 398](#).

All  $X$ -valleys and  $L$ -valleys sit in the first conduction band, C1, and are referenced as:

```
MATERIAL Silicon.conduction.C1.<valley>.min.<parameter> <value>
```

The  $\Gamma$ -valley, however, sits in the second conduction band, C2, and is referenced as:

```
MATERIAL Silicon.conduction.C2.<valley>.min.<parameter> <value>
```

Table 81 Position and orientation parameters of X-minima of conduction band

Parameter symbol	Parameter name	Description	Default	Unit
X1				
$k_0$	pos	Position within the Brillouin zone	0.85 0.0 0.0	$2\pi/a$
x	x	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
y	y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
z	z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
X2				
$k_0$	pos	Position within the Brillouin zone	-0.85 0.0 0.0	$2\pi/a$

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### Conduction Band Model

*Table 81 Position and orientation parameters of X-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$x$	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X3</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.85 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	0 1 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X4</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 -0.85 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	0 1 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X5</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.85	$2\pi/a$
$x$	X	Orientation of the x-axis	0 0 1	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 -1 0	$\langle hkl \rangle$
<b>X6</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 -0.85	$2\pi/a$

## Chapter 15: Silicon Material Model

### Conduction Band Model

*Table 81 Position and orientation parameters of X-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$x$	X	Orientation of the x-axis	0 1 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 -1 0	$\langle hkl \rangle$

*Table 82 Position and orientation parameters of L-minima of conduction band*

Parameter symbol	Parameter name	Description	Default	Unit
<b>L1</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 0.5 0.5	$2\pi/a$
$x$	X	Orientation of the x-axis	1 1 1	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 -1 2	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L2</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 0.5 0.5	$2\pi/a$
$x$	X	Orientation of the x-axis	-1 1 1	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	1 -1 2	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	1 1 0	$\langle hkl \rangle$
<b>L3</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 -0.5 0.5	$2\pi/a$
$x$	X	Orientation of the x-axis	-1 -1 1	$\langle hkl \rangle$

## Chapter 15: Silicon Material Model

### Conduction Band Model

*Table 82 Position and orientation parameters of L-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
y	Y	Orientation of the y-axis	-1 -1 -2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L4</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 -0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 -1 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$
<b>L5</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	1 1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L6</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	1 -1 -2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L7</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 -0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 -1 -1	$\langle hkl \rangle$

## Chapter 15: Silicon Material Model

### Conduction Band Model

*Table 82 Position and orientation parameters of L-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
y	Y	Orientation of the y-axis	-1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 1 0	$\langle hkl \rangle$
<b>L8</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 -0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 -1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$

*Table 83 Position and orientation parameters of  $\Gamma$ -minimum of conduction band*

Parameter symbol	Parameter name	Description	Default	Unit
<b>G</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.0	$2\pi/a$
x	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$

## Parameters

To change the default parameter values of the valley minima models, listed in the following tables, for each valley listed in [Table 80](#), use the following input file syntax:

```
MATERIAL Silicon.conduction.C1.<valley>.<parameter> <value>
```

### Note:

By default, all  $X$ -minima have the same parameter values, and all  $L$ -minima have the same parameter values.

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### Conduction Band Model

*Table 84 Parameters of X-valley model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Minima with respect to band edge	0.0	eV
$m_x$	mx	Longitudinal effective mass	0.9163	$m_e$
$m_y$	my	Transverse effective mass	0.1982	$m_e$
$m_z$	mz	Transverse effective mass	0.1982	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.5	—
$\Xi_u$	xi_u	Uniaxial deformation potential	9.16	eV
$\Xi_d$	xi_d	Dilatation deformation potential	4.18	eV
$\Xi'_u$	xi_u_prime	Uniaxial mass deformation	7.00	eV
$M$	M	Fitting parameter for electron mass	1.2	—

*Table 85 Parameters of L-valley model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Minima with respect to band edge	1.045	eV
$m_x$	mx	Longitudinal effective mass	1.634	$m_e$
$m_y$	my	Transverse effective mass	0.126	$m_e$
$m_z$	mz	Transverse effective mass	0.126	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.3	—
$\Xi_u$	xi_u	Uniaxial deformation potential	16.14	eV

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### Conduction Band Model

*Table 85 Parameters of L-valley model (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$\Xi_d$	xi_d	Dilatation deformation potential	-0.66	eV
$\Xi'_u$	xi_u_prime	Uniaxial mass deformation	0.00	eV

*Table 86 Parameters of  $\Gamma$ -valley model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Minima with respect to band edge	2.371	eV
$m_x$	mx	Longitudinal effective mass	1.987	$m_e$
$m_y$	my	Transverse effective mass	0.229	$m_e$
$m_z$	mz	Transverse effective mass	0.229	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$\Xi_u$	xi_u	Uniaxial deformation potential	0.0	eV
$\Xi_d$	xi_d	Dilatation deformation potential	0.0	eV
$\Xi'_u$	xi_u_prime	Uniaxial mass deformation	0.0	eV

## X-Valley Scattering Mechanisms

The six  $X$ -minima define the set of scattering mechanisms listed in [Table 89](#). By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL Silicon.conduction.C1.<valley>.<mechanism> ADD
MATERIAL Silicon.conduction.C1.<valley>.<mechanism> REMOVE
```

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### Conduction Band Model

*Table 87 Scattering mechanisms for X-minima*

Scattering mechanism	X1	X2	X3	X4	X5	X6
	Mechanism name					
Acoustic Phonon (long)	acl	acl	acl	acl	acl	acl
Acoustic Phonon (trans)	act	act	act	act	act	act
Optical Phonon (intra)	opx	opx	opx	opx	opx	opx
Optical Phonon (inter)	g1x2	g1x1	g1x4	g1x3	g1x6	g1x5
Optical Phonon (inter)	g2x2	g2x1	g2x4	g2x3	g2x6	g2x5
Optical Phonon (inter)	g3x2	g3x1	g3x4	g3x3	g3x6	g3x5
Optical Phonon (inter)	f1x3	f1x3	f1x1	f1x1	f1x1	f1x1
Optical Phonon (inter)	f1x4	f1x4	f1x2	f1x2	f1x2	f1x2
Optical Phonon (inter)	f1x5	f1x5	f1x5	f1x5	f1x3	f1x3
Optical Phonon (inter)	f1x6	f1x6	f1x6	f1x6	f1x4	f1x4
Optical Phonon (inter)	f2x3	f2x3	f2x1	f2x1	f2x1	f2x1
Optical Phonon (inter)	f2x4	f2x4	f2x2	f2x2	f2x2	f2x2
Optical Phonon (inter)	f2x5	f2x5	f2x5	f2x5	f2x3	f2x3
Optical Phonon (inter)	f2x6	f2x6	f2x6	f2x6	f2x4	f2x4
Optical Phonon (inter)	f3x3	f3x3	f3x1	f3x1	f3x1	f3x1
Optical Phonon (inter)	f3x4	f3x4	f3x2	f3x2	f3x2	f3x2
Optical Phonon (inter)	f3x5	f3x5	f3x5	f3x5	f3x3	f3x3
Optical Phonon (inter)	f3x6	f3x6	f3x6	f3x6	f3x4	f3x4
Optical Phonon (inter)	opl1	opl1	opl1	opl1	opl1	opl1
Optical Phonon (inter)	opl2	opl2	opl2	opl2	opl2	opl2
Optical Phonon (inter)	opl3	opl3	opl3	opl3	opl3	opl3

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### Conduction Band Model

Table 87 Scattering mechanisms for X-minima (Continued)

Scattering mechanism	X1	X2	X3	X4	X5	X6
	Mechanism name					
Optical Phonon (inter)	opl4	opl4	opl4	opl4	opl4	opl4
Optical Phonon (inter)	opl5	opl5	opl5	opl5	opl5	opl5
Optical Phonon (inter)	opl6	opl6	opl6	opl6	opl6	opl6
Optical Phonon (inter)	opl7	opl7	opl7	opl7	opl7	opl7
Optical Phonon (inter)	opl8	opl8	opl8	opl8	opl8	opl8
Optical Phonon (inter)	opg	opg	opg	opg	opg	opg
Ionized Impurity	II	II	II	II	II	II
Surface Roughness	SR	SR	SR	SR	SR	SR
Remote Coulomb	RC	RC	RC	RC	RC	RC

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each *X*-minimum, listed in Table 87, have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL Silicon.conduction.C1.<valley>.<mechanism>.<parameter> <value>
```

### Inelastic Acoustic Phonon Scattering

Table 88 lists the default parameter values of intravalley inelastic *longitudinal* acoustic phonon scattering.

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Table 88 Parameters of inelastic longitudinal acoustic phonon scattering

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
		Mechanism name:	acl						
		Description	Default						
$\Delta_{ac}$	D	Acoustic deformation	2.25						eV
$v$	v	Velocity		$9.04 \times 10^3$					m/s
$c$	c	Dispersion fitting		$-2.00 \times 10^{-7}$					$m^2/s$
$i$	final	Final minima	X2	X1	X4	X3	X6	X5	—

Table 89 lists the default parameter values of intravalley inelastic *transverse* acoustic phonon scattering.

Table 89 Parameters of inelastic transverse acoustic phonon scattering

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
		Mechanism name:	act						
		Description	Default						
$\Delta_{ac}$	D	Acoustic deformation	4.5						eV
$v$	v	Velocity		$5.34 \times 10^3$					m/s
$c$	c	Dispersion fitting		$-2.26 \times 10^{-7}$					$m^2/s$
$i$	final	Final minima	X2	X1	X4	X3	X6	X5	—

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#### Optical Phonon Scattering

[Table 90](#) to [Table 95](#) list the default parameter values of intervalley g-type and f-type optical phonon scattering.

*Table 90 Parameters of intervalley g-type (1) optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
		Mechanism name:	g1x2	g1x1	g1x4	g1x3	g1x6	g1x5	
		Description	Default						
$E_{op}$	E	Phonon energy		$12.06 \times 10^{-3}$					eV
$D_{op}$	Cc	Coupling constant		$7.5 \times 10^9$					eV/m
$i$	final	Final minima	X2	X1	X4	X3	X6	X5	—

*Table 91 Parameters of intervalley g-type (2) optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
		Mechanism name:	g2x2	g2x1	g2x4	g2x3	g2x6	g2x5	
		Description	Default						
$E_{op}$	E	Phonon energy		$18.53 \times 10^{-3}$					eV
$D_{op}$	Cc	Coupling constant		$8.0 \times 10^9$					eV/m
$i$	final	Final minima	X2	X1	X4	X3	X6	X5	—

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*Table 92 Parameters of intervalley g-type (3) optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
		Mechanism name:	g3x2	g3x1	g3x4	g3x3	g3x6	g3x5	
<b>Description</b>		<b>Default</b>							
$E_{op}$	E	Phonon energy							eV
$D_{op}$	cc	Coupling constant							eV/m
$i$	final	Final minima	X2	X1	X4	X3	X6	X5	–

*Table 93 Parameters of intervalley f-type (1) optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
		Mechanism name:	f1x[3, 4, 5, 6]	f1x[1, 2, 5, 6]	f1x[1, 2, 3, 4]				
<b>Description</b>		<b>Default</b>							
$E_{op}$	E	Phonon energy							eV
$D_{op}$	cc	Coupling constant							eV/m
$i$	final	Final minima	X[3, 4, 5, 6]	X[1, 2, 5, 6]	X[1, 2, 3, 4]				–

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*Table 94 Parameters of intervalley f-type (2) optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
		Mechanism name:	f2x[3, 4, 5, 6]	f2x[1, 2, 5, 6]	f2x[1, 2, 3, 4]				
<b>Description      Default</b>									
$E_{\text{op}}$	E	Phonon energy	$47.40 \times 10^{-3}$						eV
$D_{\text{op}}$	CC	Coupling constant	$3.4 \times 10^{10}$						eV/m
$i$	final	Final minima	X[3, 4, 5, 6]	X[1, 2, 5, 6]	X[1, 2, 3, 4]				–

*Table 95 Parameters of intervalley f-type (3) optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
		Mechanism name:	f3x[3, 4, 5, 6]	f3x[1, 2, 5, 6]	f3x[1, 2, 3, 4]				
<b>Description      Default</b>									
$E_{\text{op}}$	E	Phonon energy	$59.03 \times 10^{-3}$						eV
$D_{\text{op}}$	CC	Coupling constant	$4.0 \times 10^{10}$						eV/m
$i$	final	Final minima	X[3, 4, 5, 6]	X[1, 2, 5, 6]	X[1, 2, 3, 4]				–

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### Conduction Band Model

[Table 96](#) and [Table 97](#) list the default parameter values of intervalley optical phonon scattering.

Table 96 Parameters of intervalley X to L optical phonon scattering

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
<b>Mechanism name:</b> opl[1, 2, 3, 4, 5, 6, 7, 8]									
<b>Description</b>									<b>Default</b>
$E_{op}$	E	Phonon energy	$37.16 \times 10^{-3}$						eV
$D_{op}$	Cc	Coupling constant	$2.34 \times 10^{10}$						eV/m
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]						—

Table 97 Parameters of intervalley X to  $\Gamma$  optical phonon scattering

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
<b>Mechanism name:</b> opg									
<b>Description</b>									<b>Default</b>
$E_{op}$	E	Phonon energy	$21.89 \times 10^{-3}$						eV
$D_{op}$	Cc	Coupling constant	$5.48 \times 10^{10}$						eV/m
$i$	final	Final minima	G						—

## L-Valley Scattering Mechanisms

The eight  $L$ -minima define the set of scattering mechanisms listed in [Table 98](#). By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL Silicon.conduction.C1.<valley>.<mechanism> ADD
```

```
MATERIAL Silicon.conduction.C1.<valley>.<mechanism> REMOVE
```

## Chapter 15: Silicon Material Model

### Conduction Band Model

Table 98 Scattering mechanisms for L-minima

Scattering mechanism	L1	L2	L3	L4	L5	L6	L7	L8
	Mechanism name							
Acoustic Phonon (long)	acl	acl	acl	acl	acl	acl	acl	acl
Acoustic Phonon (trans)	act	act	act	act	act	act	act	act
Optical Phonon (inter)	opl2	opl1						
Optical Phonon (inter)	opl3	opl3	opl2	opl2	opl2	opl2	opl2	opl2
Optical Phonon (inter)	opl4	opl4	opl4	opl3	opl3	opl3	opl3	opl3
Optical Phonon (inter)	opl5	opl5	opl5	opl5	opl4	opl4	opl4	opl4
Optical Phonon (inter)	opl6	opl6	opl6	opl6	opl6	opl5	opl5	opl5
Optical Phonon (inter)	opl7	opl7	opl7	opl7	opl7	opl7	opl6	opl6
Optical Phonon (inter)	opl8	opl8	opl8	opl8	opl8	opl8	opl8	opl7
Optical Phonon (inter)	opx1	opx1	opx1	opx1	opx1	opx1	opx1	opx1
Optical Phonon (inter)	opx2	opx2	opx2	opx2	opx2	opx2	opx2	opx2
Optical Phonon (inter)	opx3	opx3	opx3	opx3	opx3	opx3	opx3	opx3
Optical Phonon (inter)	opx4	opx4	opx4	opx4	opx4	opx4	opx4	opx4
Optical Phonon (inter)	opx5	opx5	opx5	opx5	opx5	opx5	opx5	opx5
Optical Phonon (inter)	opx6	opx6	opx6	opx6	opx6	opx6	opx6	opx6
Optical Phonon (inter)	opg	opg	opg	opg	opg	opg	opg	opg
Ionized Impurity	II	II	II	II	II	II	II	II
Surface Roughness	SR	SR	SR	SR	SR	SR	SR	SR
Remote Coulomb	RC	RC	RC	RC	RC	RC	RC	RC

## Chapter 15: Silicon Material Model

### Conduction Band Model

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each  $L$ -minimum, listed in [Table 98](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL Silicon.conduction.C1.<valley>.<mechanism>.<parameter> <value>
```

### Inelastic Acoustic Phonon Scattering

[Table 99](#) lists the default parameter values of intravalley inelastic *longitudinal* acoustic phonon scattering.

*Table 99 Parameters of inelastic longitudinal acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
Mechanism name: acl											
Description											Default
$\Delta_{ac}$	D	Acoustic deformation	2.25								eV
$v$	v	Velocity		$9.04 \times 10^3$							m/s
$c$	c	Dispersion fitting		$-2.00 \times 10^{-7}$							$m^2/s$
$i$	final	Final minima	L1	L2	L3	L4	L5	L6	L7	L8	—

[Table 100](#) lists the default parameter values of intravalley inelastic *transverse* acoustic phonon scattering.

*Table 100 Parameters of inelastic transverse acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
Mechanism name: act											
Description											Default
$\Delta_{ac}$	D	Acoustic deformation	4.5								eV
$v$	v	Velocity		$5.34 \times 10^3$							m/s

## Chapter 15: Silicon Material Model

### Conduction Band Model

*Table 100 Parameters of inelastic transverse acoustic phonon scattering (Continued)*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	act								
<b>Description</b>											<b>Default</b>
<i>c</i>	<i>c</i>	Dispersion fitting									$\text{m}^2/\text{s}$
<i>i</i>	<i>final</i>	Final minima	L1	L2	L3	L4	L5	L6	L7	L8	—

### Optical Phonon Scattering

[Table 101](#) to [Table 103](#) list the default parameter values of intervalley optical phonon scattering.

*Table 101 Parameters of intervalley L to X optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opx[1, 2, 3, 4, 5, 6]								
<b>Description</b>											<b>Default</b>
$E_{\text{op}}$	<i>E</i>	Phonon energy									$\text{eV}$
$D_{\text{op}}$	<i>Cc</i>	Coupling constant									$\text{eV}/\text{m}$
<i>i</i>	<i>final</i>	Final minima	X[1, 2, 3, 4, 5, 6]								—

*Table 102 Parameters of intervalley L to L optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opl[1, 2, 3, 4, 5, 6, 7, 8]								
<b>Description</b>											<b>Default</b>
$E_{\text{op}}$	<i>E</i>	Phonon energy									$\text{eV}$
$D_{\text{op}}$	<i>Cc</i>	Coupling constant									$\text{eV}/\text{m}$

## Chapter 15: Silicon Material Model

### Conduction Band Model

Table 102 Parameters of intervalley L to L optical phonon scattering (Continued)

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opl[1, 2, 3, 4, 5, 6, 7, 8]								
		Description	Default								
i	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]								-

Table 103 Parameters of intervalley L to  $\Gamma$  optical phonon scattering

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opg								
		Description	Default								
$E_{\text{op}}$	E	Phonon energy	20.90	$\times 10^{-3}$							eV
$D_{\text{op}}$	cc	Coupling constant	5.01	$\times 10^{10}$							eV/m
i	final	Final minima	G								-

## $\Gamma$ -Valley Scattering Mechanisms

The  $\Gamma$ -minimum defines the set of scattering mechanisms listed in Table 104. By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL Silicon.conduction.C2.G.<mechanism> ADD
MATERIAL Silicon.conduction.C2.G.<mechanism> REMOVE
```

Table 104 Scattering mechanisms for  $\Gamma$ -minimum

Scattering mechanism	Mechanism name
Acoustic Phonon (long)	acl
Acoustic Phonon (trans)	act

## Chapter 15: Silicon Material Model

### Conduction Band Model

Table 104 Scattering mechanisms for  $\Gamma$ -minimum (Continued)

Scattering mechanism	Mechanism name
Optical Phonon (inter)	opl1
Optical Phonon (inter)	opl2
Optical Phonon (inter)	opl3
Optical Phonon (inter)	opl4
Optical Phonon (inter)	opl5
Optical Phonon (inter)	opl6
Optical Phonon (inter)	opl7
Optical Phonon (inter)	opl8
Optical Phonon (inter)	opx1
Optical Phonon (inter)	opx2
Optical Phonon (inter)	opx3
Optical Phonon (inter)	opx4
Optical Phonon (inter)	opx5
Optical Phonon (inter)	opx6
Ionized Impurity	II
Surface Roughness	SR
Remote Coulomb	RC

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for the  $\Gamma$ -minimum, listed in [Table 104](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL Silicon.conduction.C2.G.<mechanism>. <parameter> <value>
```

## Chapter 15: Silicon Material Model

Conduction Band Model

### Inelastic Acoustic Phonon Scattering

**Table 105** lists the default parameter values of intravalley inelastic *longitudinal* acoustic phonon scattering.

*Table 105 Parameters of inelastic longitudinal acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	acl	
		Description	Default	
$\Delta_{ac}$	D	Acoustic deformation	2.25	eV
v	v	Velocity	$9.04 \times 10^3$	m/s
c	c	Dispersion fitting	$-2.00 \times 10^{-7}$	$\text{m}^2/\text{s}$
i	final	Final minima	G	—

**Table 106** lists the default parameter values of intravalley inelastic *transverse* acoustic phonon scattering.

*Table 106 Parameters of inelastic transverse acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	act	
		Description	Default	
$\Delta_{ac}$	D	Acoustic deformation	4.5	eV
v	v	Velocity	$5.34 \times 10^3$	m/s
c	c	Dispersion fitting	$-2.26 \times 10^{-7}$	$\text{m}^2/\text{s}$
i	final	Final minima	G	—

## Chapter 15: Silicon Material Model

### Conduction Band Model

#### Optical Phonon Scattering

[Table 107](#) and [Table 108](#) list the default parameter values of intervalley optical phonon scattering.

*Table 107 Parameters of intervalley  $\Gamma$  to X optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	opx[1, 2, 3, 4, 5, 6]	
		Description	Default	
$E_{\text{op}}$	E	Phonon energy	$21.89 \times 10^{-3}$	eV
$D_{\text{op}}$	Cc	Coupling constant	$5.48 \times 10^{10}$	eV/m
$i$	final	Final minima	X[1, 2, 3, 4, 5, 6]	—

*Table 108 Parameters of intervalley  $\Gamma$  to L optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	opl[1, 2, 3, 4, 5, 6, 7, 8]	
		Description	Default	
$E_{\text{op}}$	E	Phonon energy	$21.89 \times 10^{-3}$	eV
$D_{\text{op}}$	Cc	Coupling constant	$5.48 \times 10^{10}$	eV/m
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]	—

---

## Ionized Impurity Scattering

Ionized impurity scattering is defined for each valley in a conduction band and is treated as an intravalley process by default, so that the final valley after scattering is the same as the initial valley.

*Table 109 Parameters of ionized impurity scattering*

Parameter symbol	Parameter name	Valley name:	All valleys	Unit
		Mechanism name:	II	
		Description	Default	
<i>i</i>	final	Final minimum	Same as initial minimum	–

## Ionized Impurity Empirical Rate Factor

The ionized impurity scattering model includes a scaling factor for the empirical correction of the calculated scattering rate as a function of doping density.

To redefine the default empirical factor, use the following input file syntax:

```
MATERIAL Silicon.conduction.IIfac N <Nvalue> [<Nvalue2>] <rule> <value>
```

Here, **IIfac** is a piecewise interpolation parameter that defines a correction factor **<value>** for a value **<Nvalue>** of the doping concentration **N**. The interpolation model used to return values between specified densities is given by **<rule>**, which might require an upper bound of the density [**<Nvalue2>**]. For a description of the interpolation parameter type, see [Interpolation Methods on page 301](#).

By default, the empirical correction for ionized impurity is 1.0. However, for electrons in silicon, a non-unity default value is provided to best match experimental low-field concentration-dependent mobility.

---

## Surface Roughness Scattering

**Table 110** lists the default parameter values of surface roughness scattering. These parameters apply to all valleys and to all equivalent surface orientations.

*Table 110 Parameters of surface roughness scattering*

Parameter symbol	Parameter name	Mechanism name:	SR		Unit
		Description	Default		
$\Delta$	rms	RMS amplitude	0.33	0.65	nm
$L_c$	l	Correlation length	1.00	1.0	nm
$\langle hkl \rangle$	orient	Surface orientation	(001)	(110)	–
$i$	carrier	Carrier type	electrons	electrons	–

---

## Remote Coulomb Scattering

**Table 111** lists the default parameter values of remote Coulomb scattering, which is treated as an intravalley process. These parameters apply to all valleys.

*Table 111 Parameters of remote Coulomb scattering*

Parameter symbol	Parameter name	Mechanism name:	RC		Unit
		Description	Default		
$z_d$	zd	Depth of charge centroid	1.5		nm
$E_0$	e0	Minimum energy for tabulating rate	0		eV
$N_0$	n0	Minimum screening density	$5 \times 10^{15}$		$\text{cm}^{-3}$
$i$	final	Final minimum	Same as initial minimum		–

---

To define the interface charge density for remote Coulomb scattering, follow the descriptions in [Defining Interface Models on page 217](#). By default, no interface charge is applied.

## Chapter 15: Silicon Material Model

### Valence Band Model

## Valence Band Model

This section describes the valence band model.

### Band Edge Parameters

To change the default parameter values of the valence band container model, listed in [Table 112](#), use the following input file syntax:

```
MATERIAL Silicon.valence.<parameter> <value>
```

*Table 112 Parameters of valence band container model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Valence band energy with respect to vacuum	5.1969	eV
$m_{dg_x}$	$dgx$	Hole density gradient effective x-mass	0.5	$m_e$
$m_{dg_y}$	$dgy$	Hole density gradient effective y-mass	0.5	$m_e$
$m_{dg_z}$	$dgz$	Hole density gradient effective z-mass	0.5	$m_e$
k·p band structure model parameters				
$L$	$L-kp$	Valence band parameter	-6.53	$\hbar^2/2m$
$M$	$M-kp$	Valence band parameter	-4.64	$\hbar^2/2m$
$N$	$N-kp$	Valence band parameter	-8.32	$\hbar^2/2m$
$l$	$l-defpot$	Valence deformation potential	-2.3	eV
$m$	$m-defpot$	Valence deformation potential	4.3	eV
$n$	$n-defpot$	Valence deformation potential	-9.18	eV
$\Delta_{sso}$	$dsso$	Spin-orbit split energy	0.044	eV

## Chapter 15: Silicon Material Model

### Valence Band Model

To change the default parameter values of the valence bands in the container model, listed in [Table 113](#), use the following input file syntax:

```
MATERIAL Silicon.valence.<band>.<parameter> <value>
```

*Table 113 Parameters of valence band model*

Parameter symbol	Parameter name	Description	Default	Unit
<b>Heavy hole (HH) band</b>				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.0	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	6kp	—
<b>Light hole (LH) band</b>				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.0	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	6kp	—
<b>Spin split-off (SSO) band</b>				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.044	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	6kp	—

## Mobility Models

The valence band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models together with some phenomenological enhancement factors.

### Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 114](#), use the following input file syntax:

```
MATERIAL Silicon.valence.constant.<parameter> <value>
```

## Chapter 15: Silicon Material Model

### Valence Band Model

Table 114 Parameters of constant mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	470.5	$\text{cm}^2/\text{Vs}$
$\zeta$	zeta	Fitting parameter	2.2	—

## Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 115](#), use the following input file syntax:

```
MATERIAL Silicon.valence.Arora.<parameter> <value>
```

Table 115 Parameters of Arora mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min}$	mumin	Minimum mobility	54.3	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	461.3	$\text{cm}^2/\text{Vs}$
$N_0$	n0	Reference concentration	$2.35 \times 10^{17}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.88	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.33	—
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

## Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 116](#), use the following input file syntax:

```
MATERIAL Silicon.valence.Masetti.<parameter> <value>
```

## Chapter 15: Silicon Material Model

### Valence Band Model

*Table 116 Parameters of Masetti mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min 1}$	mumin1	Minimum mobility	44.9	$\text{cm}^2/\text{Vs}$
$\mu_{\min 2}$	mumin2	Minimum mobility	0.0	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	470.5	$\text{cm}^2/\text{Vs}$
$\mu_1$	mul	Maximum mobility	29.0	$\text{cm}^2/\text{Vs}$
$C_r$	cr	Reference concentration	$2.23 \times 10^{17}$	$\text{cm}^{-3}$
$C_s$	cs	Reference solid solubility concentration	$6.10 \times 10^{20}$	$\text{cm}^{-3}$
$p_c$	pc	Reference concentration	$9.23 \times 10^{16}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.719	—
$\beta$	beta	Fitting parameter	2.0	—
$\zeta$	zeta	Fitting parameter	2.2	—

## Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 117](#), use the following input file syntax:

```
MATERIAL Silicon.valence.Yamaguchi.<parameter> <value>
```

*Table 117 Parameters of Yamaguchi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

## Chapter 15: Silicon Material Model

### Valence Band Model

## Perpendicular Field: Lombardi Mobility Model

To change the default parameter values of the Lombardi mobility model, listed in [Table 118](#), use the following input file syntax:

```
MATERIAL Silicon.valence.Lombardi.<parameter> <value>
```

*Table 118 Parameters of Lombardi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
A	a	Fitting parameter	2.0	—
B	b	Fitting parameter	$9.925 \times 10^6$	cm/s
C	c	Fitting parameter	$2.947 \times 10^3$	$\text{cm}^{5/3} \text{V}^{-2/3} \text{s}^{-1}$
$\alpha$	alpha	Fitting parameter	0.0	$\text{cm}^3$
$\delta$	delta	Fitting parameter	$2.05 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$2.05 \times 10^{30}$	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	1.0	—
$\lambda$	lambda	Fitting parameter	0.0317	—
v	nu	Fitting parameter	1.0	—
$N_0$	n0	Fitting parameter	1.0	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	1.0	$\text{cm}^{-3}$
$l_{\text{crit}}$	lcrit	Critical length	$1 \times 10^{-6}$	cm

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in [Table 119](#), use the following input file syntax:

```
MATERIAL Silicon.valence.Caughey.<parameter> <value>
```

## Chapter 15: Silicon Material Model

### Valence Band Model

Table 119 Parameters of Caughey–Thomas mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$8.37 \times 10^6$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	0.52	—
$\beta_0$	beta0	Fitting parameter	1.213	—
$\beta_{\text{exp}}$	bexp	Fitting parameter	0.17	—
$\alpha$	alpha	Fitting parameter	0.0	—

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 120](#). To change the default mobility model, use the following input file syntax:

```
MATERIAL Silicon.valence.mobility.<model> <value>
```

Table 120 Parameters of default mobility model

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley valence band model consists of the valley minima listed in [Table 121](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL Silicon.valence.<band>.<valley> REMOVE
```

### Note:

The valence band analytic valley approximation is used only as a way to define density-of-states for drift-diffusion simulations and to define the valley minima in response to stress.

## Chapter 15: Silicon Material Model

### Valence Band Model

Table 121 Names of valence band minima

Valence band minimum	Band name	Valley name
Heavy hole	HH	vhh
Light hole	LH	vlh
Spin split-off	SSO	vsso

## Position and Orientation

The position and orientation of the HH, LH, and SSO valley minima are identical. [Table 122](#) shows the default values. To change the default values, use the following input file syntax:

```
MATERIAL Silicon.valence.<band>.<valley>.min.<parameter> <value>
```

Table 122 Position and orientation parameters of HH, LH, and SSO valley minima

Parameter symbol	Parameter name	Description	Default	Unit
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.0	$2\pi/a$
x	x	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
y	y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
z	z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$

## Parameters

To change the valley minima model parameters, listed in [Table 123](#), for each valley listed in [Table 121](#), use the following input file syntax:

```
MATERIAL Silicon.valence.<band>.<valley>.parameters <value>
```

Table 123 Parameters of valence band minima

Parameter symbol	Parameter name	Description	Default	Unit
<b>Heavy hole (HH) band</b>				
E	E	Minima with respect to band edge	0.0	eV

## Chapter 15: Silicon Material Model

### Valence Band Model

Table 123 Parameters of valence band minima (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$m_x$	mx	Longitudinal effective mass	0.989	$m_e$
$m_y$	my	Transverse effective mass	0.989	$m_e$
$m_z$	mz	Transverse effective mass	0.989	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	-7.736	eV
<b>Light hole (LH) band</b>				
$E$	E	Minima with respect to band edge	0.0	eV
$m_x$	mx	Longitudinal effective mass	0.4008	$m_e$
$m_y$	my	Transverse effective mass	0.4008	$m_e$
$m_z$	mz	Transverse effective mass	0.4008	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	-7.736	eV
<b>Spin split-off (SSO) band</b>				
$E$	E	Minima with respect to band edge	0.044	eV
$m_x$	mx	Longitudinal effective mass	0.147	$m_e$
$m_y$	my	Transverse effective mass	0.147	$m_e$
$m_z$	mz	Transverse effective mass	0.147	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	-7.736	eV

## Heavy-Hole Band Scattering Mechanisms

The heavy-hole (HH) band defines the set of scattering mechanisms listed in [Table 124](#). By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL Silicon.valence.HH.vhh.<mechanism> ADD
```

```
MATERIAL Silicon.valence.HH.vhh.<mechanism> REMOVE
```

*Table 124 Scattering mechanisms for heavy-hole band*

Scattering mechanism	Mechanism name
Acoustic Phonon (long)	achhl
Optical Phonon (inter)	ophh
Optical Phonon (inter)	ophl
Optical Phonon (inter)	ophs
Ionized Impurity	II
Surface Roughness	SR
Remote Coulomb	RC

## Parameters of Scattering Mechanisms

To change the default parameter values for the scattering mechanisms listed in [Table 124](#), use the following input file syntax:

```
MATERIAL Silicon.valence.HH.vhh.<mechanism>.<parameter> <value>
```

### Inelastic Acoustic Phonon Scattering

[Table 125](#) lists the default parameter values of intraband inelastic longitudinal acoustic phonon scattering.

## Chapter 15: Silicon Material Model

### Valence Band Model

*Table 125 Parameters of inelastic longitudinal acoustic phonon scattering*

Parameter symbol	Parameter name	Band name:	HH	Unit
		Mechanism name:	achhl	
		Description	Default	
$\Delta_{ac}$	D	Acoustic deformation	7.10	eV
v	v	Velocity	$9.04 \times 10^3$	m/s
c	c	Dispersion fitting	$-2.00 \times 10^{-7}$	$\text{m}^2/\text{s}$
i	final	Final band	HH	—

### Optical Phonon Scattering

[Table 126](#) lists the default parameter values of interband optical phonon scattering.

*Table 126 Parameters of interband optical phonon scattering*

Parameter symbol	Parameter name	Band name:	HH		Unit
		Mechanism name:	ophh	ophl	ophs
		Description	Default		
$E_{op}$	E	Phonon energy	$63.33 \times 10^{-3}$		eV
$D_{op}$	cc	Coupling constant	$1.05 \times 10^{11}$		eV/m
i	final	Final band	HH	LH	SSO

### Light-Hole Band Scattering Mechanisms

The light-hole (LH) band defines the set of scattering mechanisms listed in [Table 127](#). By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL Silicon.valence.LH.vlh.<mechanism> ADD
```

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### Valence Band Model

```
MATERIAL Silicon.valence.LH.vlh.<mechanism> REMOVE
```

Table 127 Scattering mechanisms for light-hole band

Scattering mechanism	Mechanism name
Acoustic Phonon (long)	acIII
Optical Phonon (inter)	oplh
Optical Phonon (inter)	opll
Optical Phonon (inter)	opls
Ionized Impurity	II
Surface Roughness	SR
Remote Coulomb	RC

## Parameters of Scattering Mechanisms

To change the default parameter values for the scattering mechanisms listed in [Table 127](#), use the following input file syntax:

```
MATERIAL Silicon.valence.LH.vlh.<mechanism>.<parameter> <value>
```

### Inelastic Acoustic Phonon Scattering

[Table 128](#) lists the default parameter values of intraband inelastic longitudinal acoustic phonon scattering.

Table 128 Parameters of inelastic longitudinal acoustic phonon scattering

Parameter symbol	Parameter name	Band name:	LH	Unit
		Mechanism name:	acIII	
		Description	Default	
$\Delta_{ac}$	D	Acoustic deformation	7.10	eV
$v$	v	Velocity	$9.04 \times 10^3$	m/s
$c$	c	Dispersion fitting	$-2.00 \times 10^{-7}$	$\text{m}^2/\text{s}$

## Chapter 15: Silicon Material Model

### Valence Band Model

*Table 128 Parameters of inelastic longitudinal acoustic phonon scattering (Continued)*

Parameter symbol	Parameter name	Band name:	LH	Unit
		Mechanism name:	acIII	
<b>Description</b>		<b>Default</b>		
<i>i</i>	final	Final band	LH	–

### Optical Phonon Scattering

[Table 129](#) lists the default parameter values of interband optical phonon scattering.

*Table 129 Parameters of interband optical phonon scattering*

Parameter symbol	Parameter name	Band name:	LH	Unit
		Mechanism name:	ophi opll opis	
<b>Description</b>		<b>Default</b>		
$E_{op}$	E	Phonon energy	$63.33 \times 10^{-3}$	eV
$D_{op}$	cc	Coupling constant	$1.05 \times 10^{11}$	eV/m
<i>i</i>	final	Final band	HH LH SSO	–

---

### Spin Split-Off Band Scattering Mechanisms

The spin split-off (SSO) band defines the set of scattering mechanisms listed in [Table 130](#). By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL Silicon.valence.SSO.vssO.<mechanism> ADD
```

```
MATERIAL Silicon.valence.SSO.vssO.<mechanism> REMOVE
```

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### Valence Band Model

Table 130 Scattering mechanisms for spin split-off band

Scattering mechanism	Mechanism name
Acoustic Phonon (long)	acssl
Optical Phonon (inter)	opsh
Optical Phonon (inter)	opsl
Optical Phonon (inter)	opss
Ionized Impurity	II
Surface Roughness	SR
Remote Coulomb	RC

## Parameters of Scattering Mechanisms

To change the default parameter values for the scattering mechanisms listed in [Table 130](#), use the following input file syntax:

```
MATERIAL Silicon.valence.SSO.vssO.<mechanism>.<parameter> <value>
```

### Inelastic Acoustic Phonon Scattering

[Table 131](#) lists the default parameter values of intraband inelastic longitudinal acoustic phonon scattering.

Table 131 Parameters of inelastic longitudinal acoustic phonon scattering

Parameter symbol	Parameter name	Band name:	SSO	Unit	
		Mechanism name: acssl			
		Description Default			
$\Delta_{ac}$	D	Acoustic deformation	7.10	eV	
v	v	Velocity	$9.04 \times 10^3$	m/s	
c	c	Dispersion fitting	$-2.00 \times 10^{-7}$	$\text{m}^2/\text{s}$	
i	final	Final band	SSO	—	

## Chapter 15: Silicon Material Model

### Valence Band Model

#### Optical Phonon Scattering

Table 132 lists the default parameter values of interband optical phonon scattering.

Table 132 Parameters of interband optical phonon scattering

Parameter symbol	Parameter name	Band name:	SSO			Unit
		Mechanism name:	opsh	opsi	opss	
		Description	Default			
$E_{op}$	E	Phonon energy	$63.33 \times 10^{-3}$			eV
$D_{op}$	cc	Coupling constant	$5.045 \times 10^{10}$			eV/m
$i$	final	Final band	HH	LH	SSO	–

#### Ionized Impurity Scattering

Ionized impurity scattering is defined for each valley in a valence band and is treated as an intravalley process by default, so that the final valley after scattering is the same as the initial valley.

Table 133 Parameters of ionized impurity scattering

Parameter symbol	Parameter name	Valley name:	All valleys		Unit
		Mechanism name:	II		
		Description	Default		
$i$	final	Final minimum	Same as initial minimum		–

#### Ionized Impurity Empirical Rate Factor

The ionized impurity scattering model includes a scaling factor for the empirical correction of the calculated scattering rate as a function of doping density.

To redefine the default empirical factor, use the following input file syntax:

```
MATERIAL Silicon.valence.IIfac N <Nvalue> [<Nvalue2>] <rule> <value>
```

Here, **IIfac** is a piecewise interpolation parameter that defines a correction factor **<value>** for a value **<Nvalue>** of the doping concentration **N**. The interpolation model used to return

## Chapter 15: Silicon Material Model

### Valence Band Model

values between specified densities is given by `<rule>`, which might require an upper bound of the density [`<Nvalue2>`]. For a description of the interpolation parameter type, see [Interpolation Methods on page 301](#).

By default, the empirical correction for ionized impurity is 1.0. However, for holes in silicon, a non-unity default value is provided to best match experimental low-field concentration-dependent mobility.

---

## Surface Roughness Scattering

[Table 134](#) lists the default parameter values of surface roughness scattering. These parameters apply to all valleys and to all equivalent surface orientations.

*Table 134 Parameters of surface roughness scattering*

Parameter symbol	Parameter name	Mechanism name:	SR		Unit
		Description	Default		
$\Delta$	rms	RMS amplitude	0.70	0.10	nm
$L_c$	l	Correlation length	2.00	0.30	nm
$\langle hkl \rangle$	orient	Surface orientation	(001)	(110)	—
$i$	carrier	Carrier type	holes	holes	—

---

## Remote Coulomb Scattering

[Table 135](#) lists the default parameter values of remote Coulomb scattering, which is treated as an intravalley process. These parameters apply to all valleys.

*Table 135 Parameters of remote Coulomb scattering*

Parameter symbol	Parameter name	Mechanism name:	RC		Unit
		Description	Default		
$z_d$	zd	Depth of charge centroid	1.5		nm
$E_0$	e0	Minimum energy for tabulating rate	0		eV
$N_0$	n0	Minimum screening density	$5 \times 10^{15}$		$\text{cm}^{-3}$

## Chapter 15: Silicon Material Model

### Simulation Results

Table 135 Parameters of remote Coulomb scattering (Continued)

Parameter symbol	Parameter name	Mechanism name:	RC	Unit
		Description	Default	
$i$	final	Final minimum	Same as initial minimum	–

To define the interface charge density for remote Coulomb scattering, follow the descriptions in [Defining Interface Models on page 217](#). By default, no interface charge is applied.

---

## Simulation Results

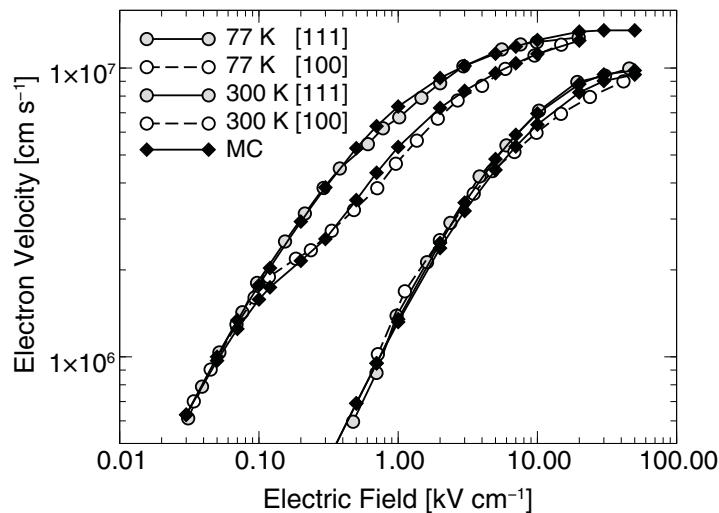
This section presents various simulation results for the silicon material model.

---

### Velocity-Field Characteristics

[Figure 40](#) shows the velocity-field characteristics for electrons in silicon at 77 K and 300 K, with the electric field applied along the  $\langle 100 \rangle$  and  $\langle 111 \rangle$  directions.

Figure 40 Calibrated electron velocity-field characteristics for silicon compared to experimental measurements [1]

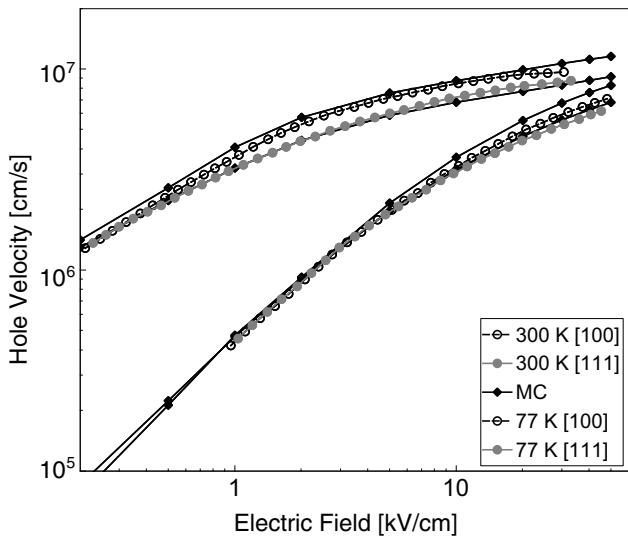


[Figure 41](#) shows the velocity-field characteristics for holes in silicon at 77 K and 300 K, with the electric field applied along the  $\langle 100 \rangle$  and  $\langle 111 \rangle$  directions.

## Chapter 15: Silicon Material Model

### Simulation Results

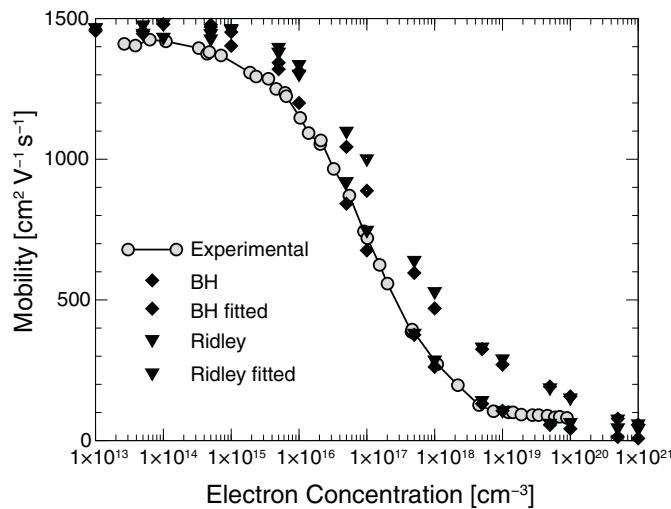
Figure 41 Calibrated hole velocity-field characteristics for silicon compared to experimental measurements [2]



## Low-Field Concentration-Dependent Mobility

Figure 42 shows the simulated low-field electron mobility in silicon at 300 K, where ionized impurity scattering is accounted for using both the Brooks–Herring and Ridley third-body exclusion scattering rates. Both the unmodified and the empirically corrected scattering rates are shown.

Figure 42 Low-field doping-dependent electron mobility in silicon compared to experimental measurement [3]

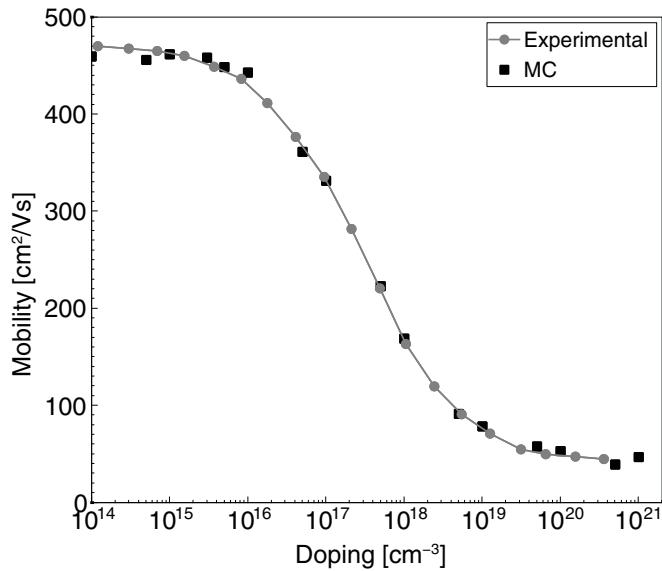


## Chapter 15: Silicon Material Model

### Simulation Results

Figure 43 shows the simulated low-field hole mobility in silicon at 300 K for both approaches to impurity scattering: Brooks–Herring (BH) and Ridley third-body exclusion (TBE).

Figure 43 Low-field doping-dependent hole mobility in silicon compared to experimental measurement [4]

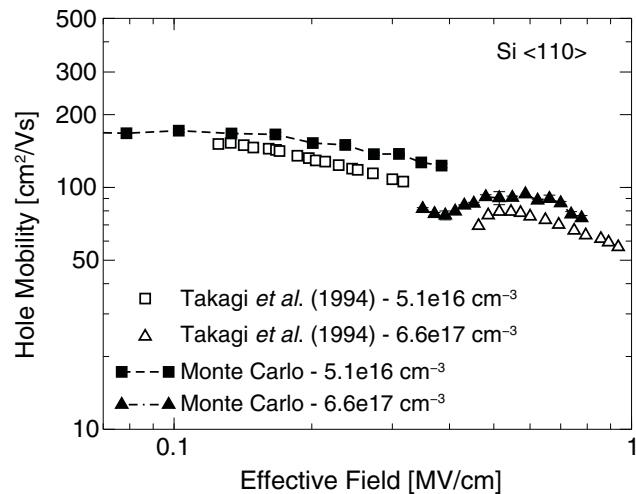


---

## Inversion Layer Mobility

Figure 44 shows the simulated low-field inversion layer mobility in silicon at 300 K, with surface roughness scattering parameters calibrated to match experimental data.

**Figure 44** Low-field hole mobility in silicon inversion layer compared to experimental measurement [5]



## References

- [1] C. Canali *et al.*, “Electron and Hole Drift Velocity Measurements in Silicon and Their Empirical Relation to Electric Field and Temperature,” *IEEE Transactions on Electron Devices*, vol. ED-22, no. 11, pp. 1045–1047, 1975.
- [2] C. Canali, G. Ottaviani, and A. Alberigi Quaranta, “Drift Velocity of Electrons and Holes and Associated Anisotropic Effects in Silicon,” *Journal of Physics and Chemistry of Solids*, vol. 32, pp. 1707–1720, 1971.
- [3] W. R. Thurber *et al.*, “Resistivity-Dopant Density Relationship for Phosphorus-Doped Silicon,” *Journal of the Electrochemical Society*, vol. 127, no. 8, pp. 1807–1812, 1980.
- [4] W. R. Thurber *et al.*, *Semiconductor Measurement Technology: The Relationship Between Resistivity and Dopant Density for Phosphorus- and Boron-Doped Silicon*, NBS Special Publication 400-64, U.S. Department of Commerce / National Bureau of Standards, Washington, DC, USA, May 1981.
- [5] S. Takagi *et al.*, “On the Universality of Inversion Layer Mobility in Si MOSFET’s: Part I—Effects of Substrate Impurity Concentration,” *IEEE Transactions on Electron Devices*, vol. 41, no. 12, pp. 2357–2362, 1994.

# 16

## Germanium Material Model

---

*This chapter describes the germanium material model.*

---

### Bulk Material Model

This section describes the bulk material model for germanium.

---

#### Parameters of Bulk Material Model

To change the default parameter values in [Table 136](#), use the following input file syntax:

```
MATERIAL Germanium.<parameter> <value>
```

*Table 136 Bulk material model parameters*

Parameter symbol	Parameter name	Description	Default	Unit
<b>Crystal lattice and orientation in simulation domain</b>				
a	a	Magnitude of lattice vector a	5.32	Å
b	b	Magnitude of lattice vector b	5.32	Å
c	c	Magnitude of lattice vector c	5.32	Å
$\alpha$	alpha	Angle between b and c	90	degree
$\beta$	beta	Angle between c and a	90	degree
$\gamma$	gamma	Angle between a and b	90	degree
$\langle hkl \rangle_x$	x	Orientation in the x-direction	1 1 0	—

## Chapter 16: Germanium Material Model

### Bulk Material Model

Table 136 Bulk material model parameters (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$\langle hkl \rangle_z$	z	Orientation in the z-direction	0 0 1	—
<b>Bulk electrical and mechanical properties</b>				
$\kappa$	permittivity	Relative dielectric constant	16.2	—
$\kappa_\infty$	k_inf	High-frequency permittivity	16.2	—
$\rho$	density	Mass density	5.32	g/cm <sup>3</sup>
$C_{11}$	c11	Elastic stiffness matrix element	132.8	GPa
$C_{12}$	c12	Elastic stiffness matrix element	46.8	GPa
$C_{44}$	c44	Elastic stiffness matrix element	66.57	GPa

## Band-to-Band Tunneling Parameters

To change the default parameter values for the Kane model, listed in [Table 137](#), use the following input file syntax:

```
MATERIAL Germanium.BTBT.<parameter> <value>
```

Table 137 Band-to-band tunneling parameters

Parameter symbol	Parameter name	Description	Default	Unit
$D_{TA}$	DTA	Acoustic phonon deformation potential	$0.80 \times 10^{10}$	eV
$\epsilon_{TA}$	epsilonTA	Acoustic phonon energy	$8.6 \times 10^{-3}$	eV

## Chapter 16: Germanium Material Model

### Conduction Band Model

---

## Conduction Band Model

This section describes the conduction band model.

---

### Band Edge Parameters

To change the default parameter values of the conduction band container model, listed in [Table 138](#), use the following input file syntax:

```
MATERIAL Germanium.conduction.<parameter> <value>
```

*Table 138 Parameters of conduction band container model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Conduction band energy with respect to vacuum	4.0	eV
$m_{dg_x}$	dgx	Electron density gradient effective x-mass	0.3	$m_e$
$m_{dg_y}$	dgy	Electron density gradient effective y-mass	0.3	$m_e$
$m_{dg_z}$	dgz	Electron density gradient effective z-mass	0.3	$m_e$

To change the default parameter values of the conduction bands in the container model, listed in [Table 139](#), use the following input file syntax:

```
MATERIAL Germanium.conduction.<band>.<parameter> <value>
```

*Table 139 Parameters of conduction band model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Conduction band energy with respect to container energy	0.0	eV
$model$	model	Model used for transport in this band	ema	—

---

## Mobility Models

The conduction band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models.

### Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 140](#), use the following input file syntax:

```
MATERIAL Germanium.conduction.constant.<parameter> <value>
```

*Table 140 Parameters of constant mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	3900	$\text{cm}^2/\text{Vs}$
$\zeta$	zeta	Fitting parameter	1.6	—

### Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 141](#), use the following input file syntax:

```
MATERIAL Germanium.conduction.Arora.<parameter> <value>
```

*Table 141 Parameters of Arora mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min}$	mumin	Minimum mobility	88.0	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	3900	$\text{cm}^2/\text{Vs}$
$N_0$	n0	Reference concentration	$1.25 \times 10^{17}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.88	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.33	—

## Chapter 16: Germanium Material Model

### Conduction Band Model

*Table 141 Parameters of Arora mobility model (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

## Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 142](#), use the following input file syntax:

```
MATERIAL Germanium.conduction.Masetti.<parameter> <value>
```

*Table 142 Parameters of Masetti mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min 1}$	mumin1	Minimum mobility	52.2	$\text{cm}^2/\text{Vs}$
$\mu_{\min 2}$	mumin2	Minimum mobility	52.2	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	3900	$\text{cm}^2/\text{Vs}$
$\mu_1$	mul	Maximum mobility	43.4	$\text{cm}^2/\text{Vs}$
$C_r$	cr	Reference concentration	$9.68 \times 10^{16}$	$\text{cm}^{-3}$
$C_s$	cs	Reference solid solubility concentration	$3.43 \times 10^{20}$	$\text{cm}^{-3}$
$p_c$	pc	Reference concentration	0.0	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.55	—
$\beta$	beta	Fitting parameter	2.0	—
$\zeta$	zeta	Fitting parameter	1.6	—

## Chapter 16: Germanium Material Model

Conduction Band Model

### Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 143](#), use the following input file syntax:

```
MATERIAL Germanium.conduction.Yamaguchi.<parameter> <value>
```

*Table 143 Parameters of Yamaguchi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

### Perpendicular Field: Lombardi Mobility Model

To change the default parameter values of the Lombardi mobility model, listed in [Table 144](#), use the following input file syntax:

```
MATERIAL Germanium.conduction.Lombardi.<parameter> <value>
```

*Table 144 Parameters of Lombardi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$A$	a	Fitting parameter	2.0	—
$B$	b	Fitting parameter	$4.75 \times 10^7$	cm/s
$C$	c	Fitting parameter	$5.80 \times 10^2$	$\text{cm}^{5/3} \text{V}^{-2/3} \text{s}^{-1}$
$\alpha$	alpha	Fitting parameter	0.0	$\text{cm}^3$
$\delta$	delta	Fitting parameter	$5.82 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$5.82 \times 10^{30}$	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	1.0	—
$\lambda$	lambda	Fitting parameter	0.125	—
$\nu$	nu	Fitting parameter	1.0	—

## Chapter 16: Germanium Material Model

Conduction Band Model

Table 144 Parameters of Lombardi mobility model (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$N_0$	n0	Fitting parameter	1.0	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	1.0	$\text{cm}^{-3}$
$l_{\text{crit}}$	lcrit	Critical length	$1 \times 10^{-6}$	cm

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in Table 145, use the following input file syntax:

```
MATERIAL Germanium.conduction.Caughey.<parameter> <value>
```

Table 145 Parameters of Caughey–Thomas mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$0.65 \times 10^7$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	0.87	–
$\beta_0$	beta0	Fitting parameter	1.109	–
$\beta_{\text{exp}}$	bexp	Fitting parameter	0.66	–
$\alpha$	alpha	Fitting parameter	0.0	–

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in Table 146. To change the default mobility model, use the following input file syntax:

```
MATERIAL Germanium.conduction.mobility.<model> <value>
```

## Chapter 16: Germanium Material Model

### Conduction Band Model

Table 146 Parameters of default mobility model

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley conduction band model consists of the valley minima listed in [Table 147](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL Germanium.conduction.<band>.<valley> REMOVE
```

Table 147 Names of conduction band minima

Conduction band minimum	Valley name
C1	
X	X1, X2, X3, X4, X5, X6
L	L1, L2, L3, L4, L5, L6, L7, L8
C2	
$\Gamma$	G

## Position and Orientation

Valley minima differ in their position and orientation, the default values of which are shown in [Table 148](#), [Table 149](#), and [Table 150](#).

To change default values, use the following input file syntax:

```
MATERIAL Germanium.conduction.c1.<valley>.min.<parameter> <value>
```

## Chapter 16: Germanium Material Model

### Conduction Band Model

Table 148 Position and orientation parameters of X-minima of conduction band

Parameter symbol	Parameter name	Description	Default	Unit
<b>X1</b>				
$k_0$	pos	Position within the Brillouin zone	0.85 0.0 0.0	$2\pi/a$
$x$	x	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X2</b>				
$k_0$	pos	Position within the Brillouin zone	-0.85 0.0 0.0	$2\pi/a$
$x$	x	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X3</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.85 0.0	$2\pi/a$
$x$	x	Orientation of the x-axis	0 1 0	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X4</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 -0.85 0.0	$2\pi/a$
$x$	x	Orientation of the x-axis	0 1 0	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$

## Chapter 16: Germanium Material Model

### Conduction Band Model

*Table 148 Position and orientation parameters of X-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
<b>X5</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.85	$2\pi/a$
$x$	x	Orientation of the x-axis	0 0 1	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	0 -1 0	$\langle hkl \rangle$
<b>X6</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 -0.85	$2\pi/a$
$x$	x	Orientation of the x-axis	0 1 0	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	0 -1 0	$\langle hkl \rangle$

*Table 149 Position and orientation parameters of L-minima of conduction band*

Parameter symbol	Parameter name	Description	Default	Unit
<b>L1</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 0.5 0.5	$2\pi/a$
$x$	x	Orientation of the x-axis	1 1 1	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	-1 -1 2	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L2</b>				

## Chapter 16: Germanium Material Model

### Conduction Band Model

*Table 149 Position and orientation parameters of L-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$k_0$	pos	Position within the Brillouin zone	-0.5 0.5 0.5	$2\pi/a$
$x$	x	Orientation of the x-axis	-1 1 1	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	1 -1 2	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	1 1 0	$\langle hkl \rangle$
<b>L3</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 -0.5 0.5	$2\pi/a$
$x$	x	Orientation of the x-axis	-1 -1 1	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	-1 -1 -2	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L4</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 -0.5 0.5	$2\pi/a$
$x$	x	Orientation of the x-axis	1 -1 1	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	-1 1 2	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$
<b>L5</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 0.5 -0.5	$2\pi/a$
$x$	x	Orientation of the x-axis	1 1 -1	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	1 1 2	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$

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Table 149 Position and orientation parameters of L-minima of conduction band (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
<b>L6</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	1 -1 -2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L7</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 -0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 -1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 1 0	$\langle hkl \rangle$
<b>L8</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 -0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 -1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$

Table 150 Position and orientation parameters of  $\Gamma$ -minimum of conduction band

Parameter symbol	Parameter name	Description	Default	Unit
<b>G</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.0	$2\pi/a$

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Table 150 Position and orientation parameters of  $\Gamma$ -minimum of conduction band (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
x	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$

## Parameters

To change the default parameter values of the valley minima models, listed in the following tables, for each valley listed in Table 147, use the following input file syntax:

```
MATERIAL Germanium.conduction.C1.<valley>.<parameter> <value>
```

### Note:

By default, all  $X$ -minima have the same parameter values, and all  $L$ -minima have the same parameter values.

Table 151 Parameters of X-valley model

Parameter symbol	Parameter name	Description	Default	Unit
E	E	Minima energy with respect to band edge	0.19953	eV
$m_x$	mx	Longitudinal effective mass	1.353	$m_e$
$m_y$	my	Transverse effective mass	0.288	$m_e$
$m_z$	mz	Transverse effective mass	0.288	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.5	—
$\Xi_u$	xi_u	Uniaxial deformation potential	9.42	eV
$\Xi_d$	xi_d	Dilatation deformation potential	-0.59	eV
$\Xi'_u$	xi_u_prime	Uniaxial mass deformation	8.07	eV

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*Table 151 Parameters of X-valley model (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$M$	<code>M</code>	Fitting parameter for electron mass	1.0	—
$\Delta$	<code>delta</code>	Fitting parameter for electron mass	0.9	eV

*Table 152 Parameters of L-valley model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	<code>E</code>	Minima energy with respect to band edge	0.0	eV
$m_x$	<code>mx</code>	Longitudinal effective mass	1.588	$m_e$
$m_y$	<code>my</code>	Transverse effective mass	0.082	$m_e$
$m_z$	<code>mz</code>	Transverse effective mass	0.082	$m_e$
$\alpha$	<code>a</code>	Valley nonparabolicity factor	0.33	—
$\Xi_u$	<code>xi_u</code>	Uniaxial deformation potential	16.7	eV
$\Xi_d$	<code>xi_d</code>	Dilatation deformation potential	-6.58	eV
$\Xi'_u$	<code>xi_u_prime</code>	Uniaxial mass deformation	0.0	eV
$M$	<code>M</code>	Fitting parameter for electron mass	0.0	—
$\Delta$	<code>delta</code>	Fitting parameter for electron mass	0.0	eV

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### Conduction Band Model

Table 153 Parameters of  $\Gamma$ -valley model

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Minima energy with respect to band edge	0.15147	eV
$m_x$	$m_x$	Longitudinal effective mass	0.037	$m_e$
$m_y$	$m_y$	Transverse effective mass	0.037	$m_e$
$m_z$	$m_z$	Transverse effective mass	0.037	$m_e$
$\alpha$	$\alpha$	Valley nonparabolicity factor	0.85	—
$\Xi_u$	$\xi_{i\_u}$	Uniaxial deformation potential	0.0	eV
$\Xi_d$	$\xi_{i\_d}$	Dilatation deformation potential	-7.0	eV
$\Xi'_u$	$\xi_{i\_u\_prime}$	Uniaxial mass deformation	0.0	eV
$M$	$M$	Fitting parameter for electron mass	0.0	—
$\Delta$	$\delta$	Fitting parameter for electron mass	0.0	eV

## X-Valley Scattering Mechanisms

The six  $X$ -minima define the set of scattering mechanisms listed in Table 154. By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL Germanium.conduction.C1.<valley>.<mechanism> ADD
```

```
MATERIAL Germanium.conduction.C1.<valley>.<mechanism> REMOVE
```

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*Table 154 Scattering mechanisms for X-minima*

Scattering mechanism	X1	X2	X3	X4	X5	X6
	Mechanism name					
Acoustic Phonon (long)	acl	acl	acl	acl	acl	acl
Acoustic Phonon (trans)	act	act	act	act	act	act
Optical Phonon (inter)	g2x2	g2x1	g2x4	g2x3	g2x6	g2x5
Optical Phonon (inter)	g3x2	g3x1	g3x4	g3x3	g3x6	g3x5
Optical Phonon (inter)	opl1	opl1	opl1	opl1	opl1	opl1
Optical Phonon (inter)	opl2	opl2	opl2	opl2	opl2	opl2
Optical Phonon (inter)	opl3	opl3	opl3	opl3	opl3	opl3
Optical Phonon (inter)	opl4	opl4	opl4	opl4	opl4	opl4
Optical Phonon (inter)	opl5	opl5	opl5	opl5	opl5	opl5
Optical Phonon (inter)	opl6	opl6	opl6	opl6	opl6	opl6
Optical Phonon (inter)	opl7	opl7	opl7	opl7	opl7	opl7
Optical Phonon (inter)	opl8	opl8	opl8	opl8	opl8	opl8
Optical Phonon (inter)	opg	opg	opg	opg	opg	opg
Ionized Impurity	II	II	II	II	II	II
Surface Roughness	SR	SR	SR	SR	SR	SR
Remote Coulomb	RC	RC	RC	RC	RC	RC

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each *X*-minimum, listed in [Table 156](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL Germanium.conduction.C1.<valley>.<mechanism>.<parameter> <value>
```

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### Inelastic Acoustic Phonon Scattering

**Table 155** lists the default parameter values of intravalley inelastic *longitudinal* acoustic phonon scattering.

*Table 155 Parameters of inelastic longitudinal acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
		Mechanism name:	acl						
		Description	Default						
$\Delta_{ac}$	D	Acoustic deformation	2.6						eV
v	v	Velocity		$5.4 \times 10^3$					m/s
c	c	Dispersion fitting		$-1.2 \times 10^{-7}$					$\text{m}^2/\text{s}$
i	final	Final minima	X1	X2	X3	X4	X5	X6	–

**Table 156** lists the default parameter values of intravalley inelastic *transverse* acoustic phonon scattering.

*Table 156 Parameters of inelastic transverse acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
		Mechanism name:	act						
		Description	Default						
$\Delta_{ac}$	D	Acoustic deformation	5.2						eV
v	v	Velocity		$3.2 \times 10^3$					m/s
c	c	Dispersion fitting		$-1.67 \times 10^{-7}$					$\text{m}^2/\text{s}$
i	final	Final minima	X1	X2	X3	X4	X5	X6	–

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### Optical Phonon Scattering

[Table 157](#) and [Table 158](#) list the default parameter values of intervalley g-type optical phonon scattering.

*Table 157 Parameters of intervalley g-type (2) optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
		Mechanism name:	g2x2	g2x1	g2x4	g2x3	g2x6	g2x5	
		<b>Description</b> <b>Default</b>							
$E_{\text{op}}$	E	Phonon energy	$37 \times 10^{-3}$						eV
$D_{\text{op}}$	cc	Coupling constant	$9.5 \times 10^{10}$						eV/m
$i$	final	Final minima	X2	X1	X4	X3	X6	X5	—

*Table 158 Parameters of intervalley g-type (3) optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
		Mechanism name:	g3x2	g3x1	g3x4	g3x3	g3x6	g3x5	
		<b>Description</b> <b>Default</b>							
$E_{\text{op}}$	E	Phonon energy	$55.89 \times 10^{-3}$						eV
$D_{\text{op}}$	cc	Coupling constant	$9.98 \times 10^{10}$						eV/m
$i$	final	Final minima	X2	X1	X4	X3	X6	X5	—

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**Table 159** and **Table 160** list the default parameter values of intervalley optical phonon scattering.

*Table 159 Parameters of intervalley X to L optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
<b>Mechanism name:</b> opl[1, 2, 3, 4, 5, 6, 7, 8]									
<b>Description</b>									<b>Default</b>
$E_{op}$	E	Phonon energy	$27.6 \times 10^{-3}$						eV
$D_{op}$	Cc	Coupling constant	$4.06 \times 10^{10}$						eV/m
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]						—

*Table 160 Parameters of intervalley X to  $\Gamma$  optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
<b>Mechanism name:</b> opg									
<b>Description</b>									<b>Default</b>
$E_{op}$	E	Phonon energy	$27.6 \times 10^{-3}$						eV
$D_{op}$	Cc	Coupling constant	$10.0 \times 10^{10}$						eV/m
$i$	final	Final minima	G						—

## L-Valley Scattering Mechanisms

The eight  $L$ -minima define the set of scattering mechanisms listed in **Table 161**. By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL Germanium.conduction.C1.<valley>. <mechanism> ADD
```

```
MATERIAL Germanium.conduction.C1.<valley>. <mechanism> REMOVE
```

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Table 161 Scattering mechanisms for L-minima

Scattering mechanism	L1	L2	L3	L4	L5	L6	L7	L8
	Mechanism name							
Acoustic Phonon (long)	acl	acl	acl	acl	acl	acl	acl	acl
Acoustic Phonon (trans)	act	act	act	act	act	act	act	act
Optical Phonon (intra)	opl1	opl2	opl3	opl4	opl5	opl6	opl7	opl8
Optical Phonon (inter)	opl2	opl1						
Optical Phonon (inter)	opl3	opl3	opl2	opl2	opl2	opl2	opl2	opl2
Optical Phonon (inter)	opl4	opl4	opl4	opl3	opl3	opl3	opl3	opl3
Optical Phonon (inter)	opl5	opl5	opl5	opl5	opl4	opl4	opl4	opl4
Optical Phonon (inter)	opl6	opl6	opl6	opl6	opl6	opl5	opl5	opl5
Optical Phonon (inter)	opl7	opl7	opl7	opl7	opl7	opl7	opl6	opl6
Optical Phonon (inter)	opl8	opl8	opl8	opl8	opl8	opl8	opl8	opl7
Optical Phonon (inter)	opl22	opl21						
Optical Phonon (inter)	opl23	opl23	opl22	opl22	opl22	opl22	opl22	opl22
Optical Phonon (inter)	opl24	opl24	opl24	opl23	opl23	opl23	opl23	opl23
Optical Phonon (inter)	opl25	opl25	opl25	opl25	opl24	opl24	opl24	opl24
Optical Phonon (inter)	opl26	opl26	opl26	opl26	opl26	opl25	opl25	opl25
Optical Phonon (inter)	opl27	opl27	opl27	opl27	opl27	opl27	opl26	opl26
Optical Phonon (inter)	opl28	opl28	opl28	opl28	opl28	opl28	opl28	opl27
Optical Phonon (intra)	opx1	opx1	opx1	opx1	opx1	opx1	opx1	opx1
Optical Phonon (inter)	opx2	opx2	opx2	opx2	opx2	opx2	opx2	opx2
Optical Phonon (inter)	opx3	opx3	opx3	opx3	opx3	opx3	opx3	opx3
Optical Phonon (inter)	opx4	opx4	opx4	opx4	opx4	opx4	opx4	opx4

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Table 161 Scattering mechanisms for L-minima (Continued)

Scattering mechanism	L1	L2	L3	L4	L5	L6	L7	L8
	Mechanism name							
Optical Phonon (inter)	opx5	opx5	opx5	opx5	opx5	opx5	opx5	opx5
Optical Phonon (inter)	opx6	opx6	opx6	opx6	opx6	opx6	opx6	opx6
Optical Phonon (inter)	opg	opg	opg	opg	opg	opg	opg	opg
Ionized Impurity	II	II	II	II	II	II	II	II
Surface Roughness	SR	SR	SR	SR	SR	SR	SR	SR
Remote Coulomb	RC	RC	RC	RC	RC	RC	RC	RC

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanism defined for each *L*-minimum, listed in Table 161, have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL Germanium.conduction.C1.<valley>.<mechanism>.<parameter> <value>
```

## Inelastic Acoustic Phonon Scattering

Table 162 lists the default parameter values of intravalley inelastic *longitudinal* acoustic phonon scattering.

Table 162 Parameters of inelastic longitudinal acoustic phonon scattering

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	acl								
		Description	Default								
$\Delta_{ac}$	D	Acoustic deformation	3.1								eV
$v$	v	Velocity	5.4×10 <sup>3</sup>								m/s
$c$	c	Dispersion fitting	–1.2×10 <sup>–7</sup>								m <sup>2</sup> /s

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Table 162 Parameters of inelastic longitudinal acoustic phonon scattering (Continued)

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	acl								
		Description	Default								
<i>i</i>	final	Final minima	L1	L2	L3	L4	L5	L6	L7	L8	–

Table 163 lists the default parameter values of intravalley inelastic transverse acoustic phonon scattering.

Table 163 Parameters of inelastic transverse acoustic phonon scattering

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	act								
		Description	Default								
$\Delta_{ac}$	D	Acoustic deformation	6.2								eV
$v$	v	Velocity	$3.2 \times 10^3$								m/s
$c$	c	Dispersion fitting	$-1.67 \times 10^{-7}$								$\text{m}^2/\text{s}$
<i>i</i>	final	Final minima	L1	L2	L3	L4	L5	L6	L7	L8	–

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### Optical Phonon Scattering

**Table 164** to **Table 168** list the default parameter values of intravalley and intervalley optical phonon scattering.

*Table 164 Parameters of intravalley optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit		
		Mechanism name:	opl[1, 2, 3, 4, 5, 6, 7, 8]										
		Description	Default										
$E_{op}$	E	Phonon energy	$37.0 \times 10^{-3}$										
$D_{op}$	Cc	Coupling constant	$5.5 \times 10^{10}$										
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]										

*Table 165 Parameters of intervalley L to X optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit		
		Mechanism name:	opx[1, 2, 3, 4, 5, 6]										
		Description	Default										
$E_{op}$	E	Phonon energy	$27.6 \times 10^{-3}$										
$D_{op}$	Cc	Coupling constant	$4.06 \times 10^{10}$										
$i$	final	Final minima	X[1, 2, 3, 4, 5, 6]										

*Table 166 Parameters of intervalley L to L (1) optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit		
		Mechanism name:	opl1[1, 2, 3, 4, 5, 6, 7, 8]										
		Description	Default										
$E_{op}$	E	Phonon energy	$27.6 \times 10^{-3}$										

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Table 166 Parameters of intervalley L to L (1) optical phonon scattering (Continued)

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opl1[1, 2, 3, 4, 5, 6, 7, 8]								
		Description	Default								
$D_{op}$	CC	Coupling constant									eV/m
$i$	final	Final minima									-

Table 167 Parameters of intervalley L to L (2) optical phonon scattering

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opl2[1, 2, 3, 4, 5, 6, 7, 8]								
		Description	Default								
$E_{op}$	E	Phonon energy									eV
$D_{op}$	CC	Coupling constant									eV/m
$i$	final	Final minima									-

Table 168 Parameters of intervalley L to  $\Gamma$  optical phonon scattering

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opg								
		Description	Default								
$E_{op}$	E	Phonon energy									eV
$D_{op}$	CC	Coupling constant									eV/m
$i$	final	Final minima									-

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## $\Gamma$ -Valley Scattering Mechanisms

The  $\Gamma$ -minimum defines the set of scattering mechanisms listed in [Table 169](#). By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL Germanium.conduction.C2.G.<mechanism> ADD
```

```
MATERIAL Germanium.conduction.C2.G.<mechanism> REMOVE
```

*Table 169 Scattering mechanisms for  $\Gamma$ -minimum*

Scattering mechanism	Mechanism name
Acoustic Phonon (long)	acl
Acoustic Phonon (trans)	act
Optical Phonon (inter)	opl1
Optical Phonon (inter)	opl2
Optical Phonon (inter)	opl3
Optical Phonon (inter)	opl4
Optical Phonon (inter)	opl5
Optical Phonon (inter)	opl6
Optical Phonon (inter)	opl7
Optical Phonon (inter)	opl8
Optical Phonon (intra)	opx1
Optical Phonon (inter)	opx2
Optical Phonon (inter)	opx3
Optical Phonon (inter)	opx4
Optical Phonon (inter)	opx5
Optical Phonon (inter)	opx6

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Table 169 Scattering mechanisms for  $\Gamma$ -minimum (Continued)

Scattering mechanism	Mechanism name
Ionized Impurity	II
Surface Roughness	SR
Remote Coulomb	RC

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for the  $\Gamma$ -minimum, listed in [Table 169](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL Germanium.conduction.C2.G.<mechanism>.<parameter> <value>
```

### Inelastic Acoustic Phonon Scattering

[Table 170](#) lists the default parameter values of intravalley inelastic *longitudinal* acoustic phonon scattering.

Table 170 Parameters of inelastic longitudinal acoustic phonon scattering

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	acl	
		Description	Default	
$\Delta_{ac}$	D	Acoustic deformation	1.2	eV
$v$	v	Velocity	$5.4 \times 10^3$	m/s
$c$	c	Dispersion fitting	$-1.2 \times 10^{-7}$	$\text{m}^2/\text{s}$
$i$	final	Final minima	G	—

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**Table 171** lists the default parameter values of intravalley inelastic *transverse acoustic phonon scattering*.

*Table 171 Parameters of inelastic transverse acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	act	
		Description	Default	
$\Delta_{ac}$	D	Acoustic deformation	2.4	eV
v	v	Velocity	$3.2 \times 10^3$	m/s
c	c	Dispersion fitting	$-1.67 \times 10^{-7}$	$m^2/s$
i	final	Final minima	G	—

### Optical Phonon Scattering

**Table 172** and **Table 173** list the default parameter values of intervalley optical phonon scattering.

*Table 172 Parameters of intervalley  $\Gamma$  to X optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	opx[1, 2, 3, 4, 5, 6]	
		Description	Default	
$E_{op}$	E	Phonon energy	$27.6 \times 10^{-3}$	eV
$D_{op}$	Cc	Coupling constant	$10.0 \times 10^{10}$	eV/m
i	final	Final minima	X[1, 2, 3, 4, 5, 6]	—

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*Table 173 Parameters of intervalley  $\Gamma$  to L optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
<b>Mechanism name:</b> opl[1, 2, 3, 4, 5, 6, 7, 8]				
Description			Default	
$E_{op}$	E	Phonon energy	$27.6 \times 10^{-3}$	eV
$D_{op}$	Cc	Coupling constant	$2.0 \times 10^{10}$	eV/m
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]	—

## Ionized Impurity Scattering

Ionized impurity scattering is defined for each valley in a conduction band and is treated as an intravalley process by default, so that the final valley after scattering is the same as the initial valley.

*Table 174 Parameters of ionized impurity scattering*

Parameter symbol	Parameter name	Valley name:	All valleys	Unit
<b>Mechanism name:</b> II				
Description			Default	
$i$	final	Final minimum	Same as initial minimum	—

## Ionized Impurity Empirical Rate Factor

The ionized impurity scattering model includes a scaling factor for the empirical correction of the calculated scattering rate as a function of doping density.

To redefine the default empirical factor, use the following input file syntax:

```
MATERIAL Germanium.conduction.IIfac N <Nvalue> [<Nvalue2>] <rule> <value>
```

Here, **IIfac** is a piecewise interpolation parameter that defines a correction factor **<value>** for a value **<Nvalue>** of the doping concentration **N**. The interpolation model used to return values between specified densities is given by **<rule>**, which might require an upper bound

## Chapter 16: Germanium Material Model

### Conduction Band Model

of the density [ $<\text{Nvalue2}>$ ]. For a description of the interpolation parameter type, see [Interpolation Methods on page 301](#).

By default, the empirical correction for ionized impurity is 1.0. However, for electrons in germanium, a non-unity default value is provided to best match experimental low-field concentration-dependent mobility.

---

## Surface Roughness Scattering

[Table 175](#) lists the default parameter values of surface roughness scattering. These parameters apply to all valleys and to all equivalent surface orientations.

*Table 175 Parameters of surface roughness scattering*

Parameter symbol	Parameter name	Mechanism name:	SR		Unit
			Description	Default	
$\Delta$	rms	RMS amplitude	0.33	0.65	nm
$L_c$	l	Correlation length	1.00	1.0	nm
$\langle \text{hkl} \rangle$	orient	Surface orientation	(001)	(110)	–
$i$	carrier	Carrier type	electrons	electrons	–

---

## Remote Coulomb Scattering

[Table 176](#) lists the default parameter values of remote Coulomb scattering, which is treated as an intravalley process. These parameters apply to all valleys.

*Table 176 Parameters of remote Coulomb scattering*

Parameter symbol	Parameter name	Mechanism name:	RC		Unit
			Description	Default	
$z_d$	$z_d$	Depth of charge centroid	1.5		nm
$E_0$	$E_0$	Minimum energy for tabulating rate	0		eV
$N_0$	$N_0$	Minimum screening density	$5 \times 10^{15}$		$\text{cm}^{-3}$

## Chapter 16: Germanium Material Model

### Valence Band Model

Table 176 Parameters of remote Coulomb scattering (Continued)

Parameter symbol	Parameter name	Mechanism name:	RC	Unit
		Description		
$i$	final	Final minimum	Same as initial minimum	–

To define the interface charge density for remote Coulomb scattering, follow the descriptions in [Defining Interface Models on page 217](#). By default, no interface charge is applied.

---

## Valence Band Model

This section describes the valence band model.

---

### Band Edge Parameters

To change the default parameter values of the valence band container model, listed in [Table 177](#), use the following input file syntax:

```
MATERIAL Germanium.valence.<parameter> <value>
```

Table 177 Parameters of valence band container model

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Valence band energy with respect to vacuum	4.664	eV
$m_{dg_x}$	$dgx$	Hole density gradient effective x-mass	0.5	$m_e$
$m_{dg_y}$	$dgy$	Hole density gradient effective y-mass	0.5	$m_e$
$m_{dg_z}$	$dgz$	Hole density gradient effective z-mass	0.5	$m_e$
<b>k-p band structure model parameters</b>				
$L$	$L-kp$	Valence band parameter	-31.58	$\hbar^2/2m$
$M$	$M-kp$	Valence band parameter	-5.1	$\hbar^2/2m$

## Chapter 16: Germanium Material Model

### Valence Band Model

*Table 177 Parameters of valence band container model (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$N$	$N\text{-kp}$	Valence band parameter	-32.1	$\hbar^2/2m$
$l$	$l\text{-defpot}$	Valence deformation potential	-2.4	eV
$m$	$m\text{-defpot}$	Valence deformation potential	4.2	eV
$n$	$n\text{-defpot}$	Valence deformation potential	-7.621	eV
$\Delta_{\text{ss}}\text{o}$	$d_{\text{ss}}\text{o}$	Spin-orbit split energy	0.296	eV

To change the default parameter values of the valence bands in the container model, listed in [Table 178](#), use the following input file syntax:

```
MATERIAL Germanium.valence.<band>.<parameter> <value>
```

*Table 178 Parameters of valence band model*

Parameter symbol	Parameter name	Description	Default	Unit
<b>Heavy hole (HH) band</b>				
$E$	$E$	Valence band energy with respect to container energy	0.0	eV
$model$	$model$	Model used for transport in this band	$6\text{kp}$	—
<b>Light hole (LH) band</b>				
$E$	$E$	Valence band energy with respect to container energy	0.0	eV
$model$	$model$	Model used for transport in this band	$6\text{kp}$	—
<b>Spin split-off (SSO) band</b>				
$E$	$E$	Valence band energy with respect to container energy	0.044	eV
$model$	$model$	Model used for transport in this band	$6\text{kp}$	—

## Mobility Models

The valence band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models together with some phenomenological enhancement factors.

### Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 179](#), use the following input file syntax:

```
MATERIAL Germanium.valence.constant.<parameter> <value>
```

*Table 179 Parameters of constant mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	1900.0	$\text{cm}^2/\text{Vs}$
$\zeta$	zeta	Fitting parameter	2.3	—

### Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 180](#), use the following input file syntax:

```
MATERIAL Germanium.valence.Arora.<parameter> <value>
```

*Table 180 Parameters of Arora mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min}$	mumin	Minimum mobility	54.3	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	muemax	Maximum mobility	1900.0	$\text{cm}^2/\text{Vs}$
$N_0$	n0	Reference concentration	$2.35 \times 10^{17}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.88	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.33	—

## Chapter 16: Germanium Material Model

### Valence Band Model

*Table 180 Parameters of Arora mobility model (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

## Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 181](#), use the following input file syntax:

```
MATERIAL Germanium.valence.Masetti.<parameter> <value>
```

*Table 181 Parameters of Masetti mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min 1}$	mumin1	Minimum mobility	60.0	$\text{cm}^2/\text{Vs}$
$\mu_{\min 2}$	mumin2	Minimum mobility	0.0	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	1900.0	$\text{cm}^2/\text{Vs}$
$\mu_1$	mul	Maximum mobility	40.0	$\text{cm}^2/\text{Vs}$
$C_r$	cr	Reference concentration	$2.0 \times 10^{17}$	$\text{cm}^{-3}$
$C_s$	cs	Reference solid solubility concentration	$1.0 \times 10^{20}$	$\text{cm}^{-3}$
$p_c$	pc	Reference concentration	$9.23 \times 10^{16}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.55	—
$\beta$	beta	Fitting parameter	2.0	—
$\zeta$	zeta	Fitting parameter	2.3	—

## Chapter 16: Germanium Material Model

### Valence Band Model

## Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 182](#), use the following input file syntax:

```
MATERIAL Germanium.valence.Yamaguchi.<parameter> <value>
```

*Table 182 Parameters of Yamaguchi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

## Perpendicular Field: Lombardi Mobility Model

To change the default parameter values of the Lombardi mobility model, listed in [Table 183](#), use the following input file syntax:

```
MATERIAL Germanium.valence.Lombardi.<parameter> <value>
```

*Table 183 Parameters of Lombardi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$A$	a	Fitting parameter	1.5	—
$B$	b	Fitting parameter	$1.993 \times 10^5$	cm/s
$C$	c	Fitting parameter	$4.875 \times 10^3$	$\text{cm}^{5/3} \text{V}^{-2/3} \text{s}^{-1}$
$\alpha$	alpha	Fitting parameter	0.0	$\text{cm}^3$
$\delta$	delta	Fitting parameter	$1.71 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$2.05 \times 10^{30}$	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	1.0	—
$\lambda$	lambda	Fitting parameter	0.0317	—
$\nu$	nu	Fitting parameter	1.0	—

## Chapter 16: Germanium Material Model

### Valence Band Model

Table 183 Parameters of Lombardi mobility model (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$N_0$	n0	Fitting parameter	1.0	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	1.0	$\text{cm}^{-3}$
$l_{\text{crit}}$	lcrit	Critical length	$1 \times 10^{-6}$	cm

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

The default parameter of the Caughey–Thomas velocity saturation mobility model, defined in [Table 184](#), can be changed by using the following input file syntax:

```
MATERIAL Germanium.valence.Caughey.<parameter> <value>
```

Table 184 Parameters of Caughey–Thomas mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$6.0 \times 10^6$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	0.52	—
$\beta_0$	beta0	Fitting parameter	1.213	—
$\beta_{\text{exp}}$	bexp	Fitting parameter	0.17	—
$\alpha$	alpha	Fitting parameter	0.0	—

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 185](#). To change the default mobility model, use the following input file syntax:

```
MATERIAL Germanium.valence.mobility.<model> <value>
```

## Chapter 16: Germanium Material Model

### Valence Band Model

Table 185 Parameters of default mobility model

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley valence band model consists of the valley minima listed in [Table 186](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL Germanium.valence.<band>.<valley> REMOVE
```

### Note:

The valence band analytic valley approximation is used only as a way to define density-of-states for drift diffusion simulations and to define the valley minima in response to stress.

Table 186 Names of valence band minima

Valence band minimum	Band name	Valley name
Heavy hole	HH	vhh
Light hole	LH	vlh
Spin split-off	SSO	vsso

## Position and Orientation

The position and orientation of the HH, LH, and SSO valley minima are identical. [Table 187](#) shows the default values. To change the default values, use the following input file syntax:

```
MATERIAL Germanium.valence.<band>.<valley>.min.<parameter> <value>
```

## Chapter 16: Germanium Material Model

### Valence Band Model

*Table 187 Position and orientation parameters of HH, LH, and SSO valley minima*

Parameter symbol	Parameter name	Description	Default	Unit
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.0	$2\pi/a$
$x$	x	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$

## Parameters

To change the valley minima model parameters, listed in [Table 188](#), for each valley listed in [Table 186](#), use the following input file syntax:

```
MATERIAL Germanium.valence.<band>.<valley>.<parameter> <value>
```

*Table 188 Parameters of valence band minima*

Parameter symbol	Parameter name	Description	Default	Unit
<b>Heavy hole (HH) band</b>				
$E$	E	Minima with respect to band edge	0.0	eV
$m_x$	mx	Longitudinal effective mass	0.353	$m_e$
$m_y$	my	Transverse effective mass	0.353	$m_e$
$m_z$	mz	Transverse effective mass	0.353	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	-0.15	eV
<b>Light hole (LH) band</b>				
$E$	E	Minima with respect to band edge	0.0	eV
$m_x$	mx	Longitudinal effective mass	0.048	$m_e$

## Chapter 16: Germanium Material Model

### Valence Band Model

Table 188 Parameters of valence band minima (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$m_y$	my	Transverse effective mass	0.048	$m_e$
$m_z$	mz	Transverse effective mass	0.048	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	-0.15	eV
<b>Spin split-off (SSO) band</b>				
$E$	E	Minima with respect to band edge	0.296	eV
$m_x$	mx	Longitudinal effective mass	0.062	$m_e$
$m_y$	my	Transverse effective mass	0.062	$m_e$
$m_z$	mz	Transverse effective mass	0.062	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	-8.15	eV

## Heavy-Hole Band Scattering Mechanisms

The heavy-hole (HH) band defines the set of scattering mechanisms listed in [Table 189](#). By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL Germanium.valence.HH.vhh.<mechanism> ADD
```

```
MATERIAL Germanium.valence.HH.vhh.<mechanism> REMOVE
```

## Chapter 16: Germanium Material Model

### Valence Band Model

Table 189 Scattering mechanisms for heavy-hole band

Scattering mechanism	Mechanism name
Acoustic Phonon (long)	achhl
Optical Phonon (inter)	ophh
Optical Phonon (inter)	ophl
Optical Phonon (inter)	ophs
Ionized Impurity	II
Surface Roughness	SR
Remote Coulomb	RC

## Parameters of Scattering Mechanisms

To change the default parameter values for the scattering mechanisms listed in [Table 189](#), use the following input file syntax:

```
MATERIAL Germanium.valence.HH.vhh.<mechanism>.<parameter> <value>
```

### Inelastic Acoustic Phonon Scattering

[Table 190](#) lists the default parameter values of intraband inelastic longitudinal acoustic phonon scattering.

Table 190 Parameters of inelastic longitudinal acoustic phonon scattering

Parameter symbol	Parameter name	Band name:	HH	Unit
		Mechanism name:	achhl	
		Description	Default	
$\Delta_{ac}$	D	Acoustic deformation	5.7	eV
v	v	Velocity	$5.4 \times 10^3$	m/s
c	c	Dispersion fitting	$-1.2 \times 10^{-7}$	$m^2/s$
i	final	Final band	HH	—

## Chapter 16: Germanium Material Model

### Valence Band Model

#### Optical Phonon Scattering

Table 191 lists the default parameter values of interband optical phonon scattering.

Table 191 Parameters of interband optical phonon scattering

Parameter symbol	Parameter name	Band name:	HH			Unit
		Mechanism name:	ophh	ophl	ophs	
		Description	Default			
$E_{\text{op}}$	E	Phonon energy	$37.01 \times 10^{-3}$			eV
$D_{\text{op}}$	cc	Coupling constant	$1.40 \times 10^{11}$			eV/m
$i$	final	Final band	HH	LH	SSO	–

#### Light-Hole Band Scattering Mechanisms

The light-hole (LH) band defines the set of scattering mechanisms listed in Table 192. By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL Germanium.valence.LH.vlh.<mechanism> ADD
```

```
MATERIAL Germanium.valence.LH.vlh.<mechanism> REMOVE
```

Table 192 Scattering mechanisms for light-hole band

Scattering mechanism	Mechanism name
Acoustic Phonon (long)	aclli
Optical Phonon (inter)	oplh
Optical Phonon (inter)	opll
Optical Phonon (inter)	opls
Ionized Impurity	II
Surface Roughness	SR

## Chapter 16: Germanium Material Model

### Valence Band Model

Table 192 Scattering mechanisms for light-hole band (Continued)

Scattering mechanism	Mechanism name
Remote Coulomb	RC

## Parameters of Scattering Mechanisms

To change the parameter values for the scattering mechanisms named in Table 192, use the following input file syntax:

```
MATERIAL Germanium.valence.LH.vlh.<mechanism>. <parameter> <value>
```

### Inelastic Acoustic Phonon Scattering

Table 193 lists the default parameter values of intraband inelastic longitudinal acoustic phonon scattering.

Table 193 Parameters of inelastic longitudinal acoustic phonon scattering

Parameter symbol	Parameter name	Band name:	LH	Unit
		Mechanism name:	aclII	
		Description	Default	
$\Delta_{ac}$	D	Acoustic deformation	5.7	eV
v	v	Velocity	$5.4 \times 10^3$	m/s
c	c	Dispersion fitting	$-1.2 \times 10^{-7}$	$\text{m}^2/\text{s}$
i	final	Final band	LH	—

## Chapter 16: Germanium Material Model

### Valence Band Model

#### Optical Phonon Scattering

Table 194 lists the default parameter values of interband optical phonon scattering.

Table 194 Parameters of interband optical phonon scattering

Parameter symbol	Parameter name	Band name:	LH			Unit
			Mechanism name:	oplh	opll	
		Description	Default			
$E_{\text{op}}$	E	Phonon energy		$37.01 \times 10^{-3}$		eV
$D_{\text{op}}$	cc	Coupling constant		$1.40 \times 10^{11}$		eV/m
$i$	final	Final band	HH	LH	SSO	-

#### Spin Split-Off Band Scattering Mechanisms

The spin split-off (SSO) band defines the set of scattering mechanisms listed in Table 195. By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL Germanium.valence.sso.vss o.<mechanism> ADD
```

```
MATERIAL Germanium.valence.sso.vss o.<mechanism> REMOVE
```

Table 195 Scattering mechanisms for spin split-off band

Scattering mechanism	Mechanism name
Acoustic Phonon (long)	acssl
Optical Phonon (inter)	opsh
Optical Phonon (inter)	opsl
Optical Phonon (inter)	opss
Ionized Impurity	II
Surface Roughness	SR

## Chapter 16: Germanium Material Model

### Valence Band Model

Table 195 Scattering mechanisms for spin split-off band (Continued)

Scattering mechanism	Mechanism name
Remote Coulomb	RC

## Parameters of Scattering Mechanisms

To change the default parameter values for the scattering mechanisms listed in [Table 195](#), use the following input file syntax:

```
MATERIAL Germanium.valence.SSO.vssso.<mechanism>. <parameter> <value>
```

### Inelastic Acoustic Phonon Scattering

[Table 196](#) lists the default parameter values of intraband inelastic longitudinal acoustic phonon scattering.

Table 196 Parameters of inelastic longitudinal acoustic phonon scattering

Parameter symbol	Parameter name	Band name:	SSO	Unit
		Mechanism name:	acssl	
		Description	Default	
$\Delta_{ac}$	D	Acoustic deformation	5.7	eV
v	v	Velocity	$5.4 \times 10^3$	m/s
c	c	Dispersion fitting	$-1.2 \times 10^{-7}$	$m^2/s$
i	final	Final band	SSO	—

## Chapter 16: Germanium Material Model

### Valence Band Model

#### Optical Phonon Scattering

Table 197 lists the default parameter values of interband optical phonon scattering.

Table 197 Parameters of interband optical phonon scattering

Parameter symbol	Parameter name	Band name:	SSO	Unit
		Mechanism name:	opsh opsl opss	
		Description	Default	
$E_{op}$	E	Phonon energy	$37.01 \times 10^{-3}$	eV
$D_{op}$	Cc	Coupling constant	$1.40 \times 10^{11}$	eV/m
$i$	final	Final band	HH LH SSO	-

#### Ionized Impurity Scattering

Ionized impurity scattering is defined for each valley in a valence band and is treated as an intravalley process by default, so that the final valley after scattering is the same as the initial valley.

Table 198 Parameters of ionized impurity scattering

Parameter symbol	Parameter name	Valley name:	All valleys	Unit
		Mechanism name:	II	
		Description	Default	
$i$	final	Final minimum	Same as initial minimum	-

#### Ionized Impurity Empirical Rate Factor

The ionized impurity scattering model includes a scaling factor for the empirical correction of the calculated scattering rate as a function of doping density.

To redefine the default empirical factor, use the following input file syntax:

```
MATERIAL Germanium.valence.IIfac N <Nvalue> [<Nvalue2>] <rule> <value>
```

Here, **IIfac** is a piecewise interpolation parameter that defines a correction factor **<value>** for a value **<Nvalue>** of the doping concentration **N**. The interpolation model used to return

## Chapter 16: Germanium Material Model

### Valence Band Model

values between specified densities is given by `<rule>`, which might require an upper bound of the density [`<Nvalue2>`]. For a description of the interpolation parameter type, see [Interpolation Methods on page 301](#).

By default, the empirical correction for ionized impurity is 1.0. However, for holes in germanium, a non-unity default value is provided to best match experimental low-field concentration-dependent mobility.

---

## Surface Roughness Scattering

[Table 199](#) lists the default parameter values of surface roughness scattering. These parameters apply to all valleys and to all equivalent surface orientations.

*Table 199 Parameters of surface roughness scattering*

Parameter symbol	Parameter name	Mechanism name:	SR		Unit
		Description	Default		
$\Delta$	rms	RMS amplitude	2.00	0.90	nm
$L_c$	l	Correlation length	3.00	2.60	nm
$\langle hkl \rangle$	orient	Surface orientation	(001)	(110)	–
$i$	carrier	Carrier type	holes	holes	–

---

## Remote Coulomb Scattering

[Table 200](#) lists the default parameter values of remote Coulomb scattering, which is treated as an intravalley process. These parameters apply to all valleys.

*Table 200 Parameters of remote Coulomb scattering*

Parameter symbol	Parameter name	Mechanism name:	RC		Unit
		Description	Default		
$z_d$	zd	Depth of charge centroid	1.5		nm
$E_0$	e0	Minimum energy for tabulating rate	0		eV
$N_0$	n0	Minimum screening density	$5 \times 10^{15}$		$\text{cm}^{-3}$

## Chapter 16: Germanium Material Model

### Simulation Results

Table 200 Parameters of remote Coulomb scattering (Continued)

Parameter symbol	Parameter name	Mechanism name:	RC	Unit
		Description		
$i$	$f_{\text{final}}$	Final minimum	Same as initial minimum	–

To define the interface charge density for remote Coulomb scattering, follow the descriptions in [Defining Interface Models on page 217](#). By default, no interface charge is applied.

---

## Simulation Results

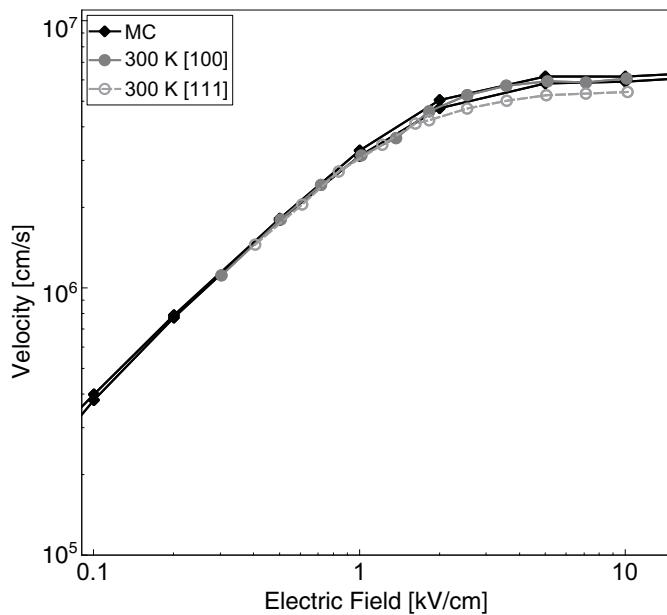
This section presents various simulation results for the germanium material model.

---

### Velocity-Field Characteristics

[Figure 45](#) shows the velocity-field characteristics for electrons in germanium at 300 K, with the electric field applied along the  $\langle 100 \rangle$  and  $\langle 111 \rangle$  directions.

Figure 45 Calibrated electron velocity-field characteristics for germanium [1]

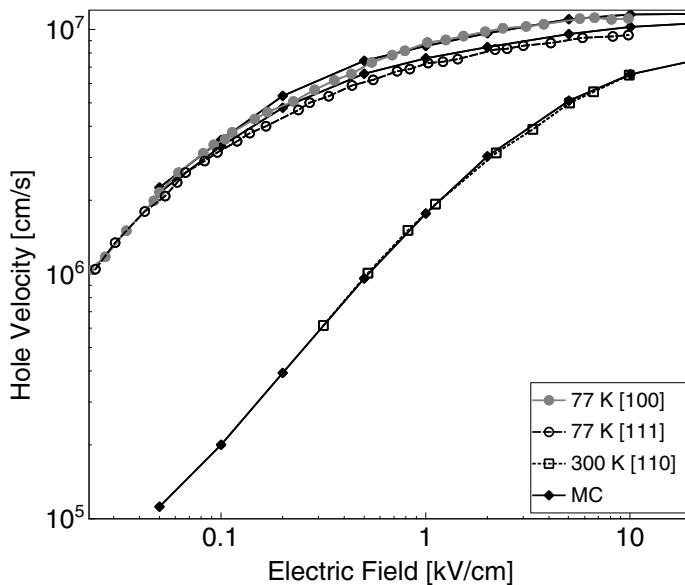


## Chapter 16: Germanium Material Model

### Simulation Results

Figure 46 shows the velocity-field characteristics for holes in germanium at 77 K and 300 K, with the electric field applied along the  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ , and  $\langle 111 \rangle$  directions.

Figure 46 Calibrated hole velocity-field characteristics for germanium [2][3]



---

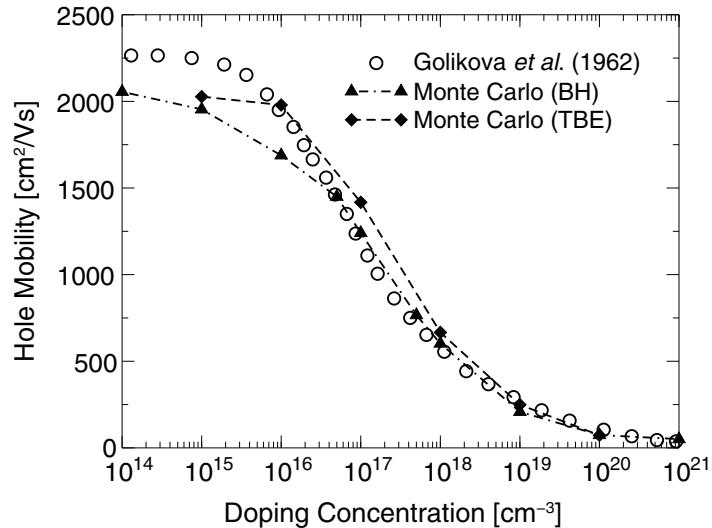
## Low-Field Concentration-Dependent Mobility

Figure 47 shows the simulated low-field hole mobility in germanium at 300 K for both approaches for impurity scattering: Brooks–Herring (BH) and Ridley’s third-body exclusion (TBE).

## Chapter 16: Germanium Material Model

### Simulation Results

Figure 47 Doping-dependent low-field hole mobility in germanium compared to experimental measurements [4]

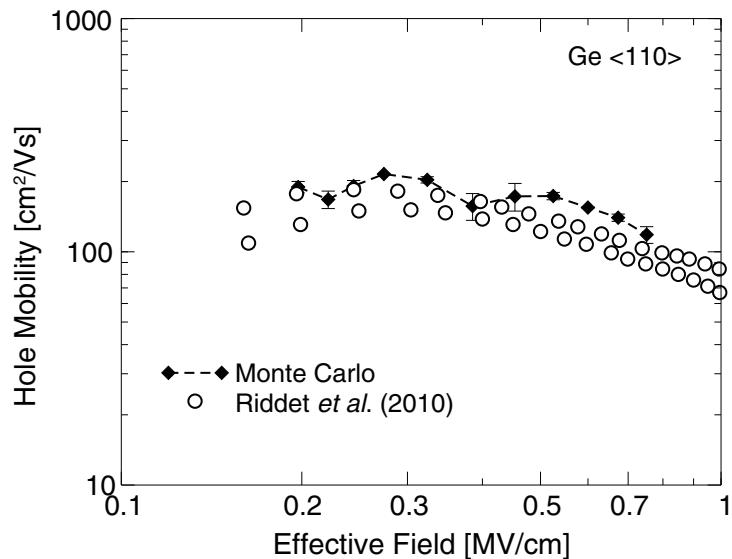


---

## Inversion Layer Mobility

Figure 48 shows the simulated low-field inversion layer mobility in germanium at 300 K, with surface roughness scattering parameters calibrated to match experimental data.

Figure 48 Low-field hole mobility in germanium inversion layer compared to experimental measurement [5]



## References

- [1] C. Jacoboni *et al.*, "Electron drift velocity and diffusivity in germanium," *Physical Review B*, vol. 24, no. 2, pp. 1014–1026, 1981.
- [2] J. P. Nougier and M. Rolland, "Mobility, Noise Temperature, and Diffusivity of Hot Holes in Germanium," *Physical Review B*, vol. 8, no. 12, pp. 5728–5737, 1973.
- [3] L. Reggiani *et al.*, "Hole drift velocity in germanium," *Physical Review B*, vol. 16, no. 6, pp. 2781–2791, 1977.
- [4] O. A. Golikova, B. Ya. Moizhes, and L. S. Stil'bans, "Hole Mobility of Germanium as a Function of Concentration and Temperature," *Soviet Physics - Solid State*, vol. 3, no. 10, pp. 2259–2265, 1962.
- [5] C. Riddet *et al.*, "Monte Carlo Simulation Study of Hole Mobility in Germanium MOS Inversion Layers," in *14th International Workshop on Computational Electronics (IWCE)*, Pisa, Italy, pp. 239–242, October 2010.

## Indium Gallium Arsenide Material Model

---

*This chapter describes the  $\text{In}_{53}\text{Ga}_{47}\text{As}$  material model.*

---

### Bulk Material Model

This section describes the bulk material model for  $\text{In}_{53}\text{Ga}_{47}\text{As}$ .

---

#### Parameters of Bulk Material Model

To change the default parameter values in [Table 201](#), use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.<parameter> <value>
```

*Table 201 Bulk material model parameters*

Parameter symbol	Parameter name	Description	Default	Unit
<b>Crystal lattice and orientation in simulation domain</b>				
$ a $	a	Magnitude of lattice vector $a$	5.868	Å
$ b $	b	Magnitude of lattice vector $b$	5.868	Å
$ c $	c	Magnitude of lattice vector $c$	5.868	Å
$\alpha$	alpha	Angle between $b$ and $c$	90	degree
$\beta$	beta	Angle between $c$ and $a$	90	degree
$\gamma$	gamma	Angle between $a$ and $b$	90	degree
$\langle hkl \rangle_x$	x	Orientation in the x-direction	1 0 0	–

## Chapter 17: Indium Gallium Arsenide Material Model

### Bulk Material Model

Table 201 Bulk material model parameters (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$\langle hkl \rangle_z$	z	Orientation in the z-direction	0 0 1	—
<b>Bulk electrical and mechanical properties</b>				
$\kappa$	permittivity	Relative dielectric constant	13.88	—
$\kappa_\infty$	k_inf	High-frequency permittivity	11.34	—
$\rho$	density	Mass density	5.50	g/cm <sup>3</sup>
$C_{11}$	c11	Elastic stiffness matrix element	100.132	GPa
$C_{12}$	c12	Elastic stiffness matrix element	49.16	GPa
$C_{44}$	c44	Elastic stiffness matrix element	48.947	GPa

## Band-to-Band Tunneling Parameters

To change the default parameter values for the Kane model, listed in [Table 202](#), use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.BTBT.<parameter> <value>
```

Table 202 Band-to-band tunneling parameters

Parameter symbol	Parameter name	Description	Default	Unit
$D_{TA}$	DTA	Acoustic phonon deformation potential	0.0	eV
$\epsilon_{TA}$	epsilonTA	Acoustic phonon energy	0.0	eV

## Chapter 17: Indium Gallium Arsenide Material Model

### Conduction Band Model

---

## Conduction Band Model

This section describes the conduction band model.

---

### Band Edge Parameters

To change the default parameter values of the conduction band container model, listed in [Table 203](#), use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.conduction.<parameter> <value>
```

*Table 203 Parameters of conduction band container model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Conduction band energy with respect to vacuum	4.5	eV
$m_{dg_x}$	$dgx$	Electron density gradient effective x-mass	0.3	$m_e$
$m_{dg_y}$	$dgy$	Electron density gradient effective y-mass	0.3	$m_e$
$m_{dg_z}$	$dgz$	Electron density gradient effective z-mass	0.3	$m_e$

To change the default parameter values of the conduction bands in the container model, listed in [Table 204](#), use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.conduction.<band>.<parameter> <value>
```

*Table 204 Parameters of conduction band model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Conduction band energy with respect to container energy	0.0	eV
$model$	$model$	Model used for transport in this band	ema	—

## Chapter 17: Indium Gallium Arsenide Material Model

### Conduction Band Model

---

## Mobility Models

The conduction band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models.

### Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 205](#), use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.conduction.constant.<parameter> <value>
```

*Table 205 Parameters of constant mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	$1.4 \times 10^4$	$\text{cm}^2/\text{Vs}$
$\zeta$	zeta	Fitting parameter	1.59	—

### Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 206](#), use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.conduction.Arora.<parameter> <value>
```

*Table 206 Parameters of Arora mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min}$	mumin	Minimum mobility	88.0	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	$1.4 \times 10^4$	$\text{cm}^2/\text{Vs}$
$N_0$	n0	Reference concentration	$1.25 \times 10^{17}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.88	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.33	—

## Chapter 17: Indium Gallium Arsenide Material Model

### Conduction Band Model

*Table 206 Parameters of Arora mobility model (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

## Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 207](#), use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.conduction.Masetti.<parameter> <value>
```

*Table 207 Parameters of Masetti mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min 1}$	mumin1	Minimum mobility	220.0	$\text{cm}^2/\text{Vs}$
$\mu_{\min 2}$	mumin2	Minimum mobility	220.0	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	$1.4 \times 10^4$	$\text{cm}^2/\text{Vs}$
$\mu_1$	mul	Maximum mobility	1.0	$\text{cm}^2/\text{Vs}$
$C_r$	cr	Reference concentration	$1.2 \times 10^{17}$	$\text{cm}^{-3}$
$C_s$	cs	Reference solid solubility concentration	0.0	$\text{cm}^{-3}$
$p_c$	pc	Reference concentration	0.0	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.5	—
$\beta$	beta	Fitting parameter	2.0	—
$\zeta$	zeta	Fitting parameter	2.1	—

## Chapter 17: Indium Gallium Arsenide Material Model

Conduction Band Model

### Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 208](#), use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.conduction.Yamaguchi.<parameter> <value>
```

*Table 208 Parameters of the Yamaguchi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

### Perpendicular Field: Lombardi Mobility Model

To change the default parameter values of the Lombardi mobility model, listed in [Table 209](#), use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.conduction.Lombardi.<parameter> <value>
```

*Table 209 Parameters of Lombardi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$A$	a	Fitting parameter	2.0	—
$B$	b	Fitting parameter	$4.75 \times 10^7$	cm/s
$C$	c	Fitting parameter	$5.80 \times 10^2$	$\text{cm}^{5/3} \text{V}^{-2/3} \text{s}^{-1}$
$\alpha$	alpha	Fitting parameter	0.0	$\text{cm}^3$
$\delta$	delta	Fitting parameter	$5.82 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$5.82 \times 10^{30}$	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	1.0	—
$\lambda$	lambda	Fitting parameter	0.125	—
$\nu$	nu	Fitting parameter	1.0	—

## Chapter 17: Indium Gallium Arsenide Material Model

### Conduction Band Model

Table 209 Parameters of Lombardi mobility model (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$N_0$	n0	Fitting parameter	1.0	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	1.0	$\text{cm}^{-3}$
$l_{\text{crit}}$	lcrit	Critical length	$1 \times 10^{-6}$	cm

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in [Table 210](#), use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.conduction.Caughey.<parameter> <value>
```

Table 210 Parameters of Caughey–Thomas mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$6.0 \times 10^6$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	0.87	—
$\beta_0$	beta0	Fitting parameter	1.109	—
$\beta_{\text{exp}}$	bexp	Fitting parameter	0.66	—
$\alpha$	alpha	Fitting parameter	0.0	—

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 211](#). To change the default mobility model, use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.conduction.mobility.<model> <value>
```

## Chapter 17: Indium Gallium Arsenide Material Model

### Conduction Band Model

Table 211 Parameters of default mobility model

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley conduction band model consists of the valley minima listed in [Table 212](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.conduction.<band>.<valley> REMOVE
```

Table 212 Names of conduction band C1 minima

Conduction band minimum	Valley name
X	X1, X2, X3, X4, X5, X6
L	L1, L2, L3, L4, L5, L6, L7, L8
$\Gamma$	G

## Position and Orientation

Valley minima differ in their position and orientation, the default values of which are shown in [Table 213](#), [Table 214](#), and [Table 215](#).

To change default values, use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.conduction.C1.<valley>.min.<parameter> <value>
```

Table 213 Position and orientation parameters of X-minima of conduction band

Parameter symbol	Parameter name	Description	Default	Unit
<b>X1</b>				
$k_0$	pos	Position within the Brillouin zone	1.0 0.0 0.0	$2\pi/a$

## Chapter 17: Indium Gallium Arsenide Material Model

### Conduction Band Model

*Table 213 Position and orientation parameters of X-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$x$	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X2</b>				
$k_0$	pos	Position within the Brillouin zone	-1.0 0.0 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X3</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 1.0 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	0 1 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X4</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 -1.0 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	0 1 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X5</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 1.0	$2\pi/a$

## Chapter 17: Indium Gallium Arsenide Material Model

### Conduction Band Model

*Table 213 Position and orientation parameters of X-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
x	X	Orientation of the x-axis	0 0 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	0 -1 0	$\langle hkl \rangle$
<b>X6</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 -1.0	$2\pi/a$
x	X	Orientation of the x-axis	0 0 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	0 -1 0	$\langle hkl \rangle$

*Table 214 Position and orientation parameters of L-minima of conduction band*

Parameter symbol	Parameter name	Description	Default	Unit
<b>L1</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 1 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L2</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 1 1	$\langle hkl \rangle$

## Chapter 17: Indium Gallium Arsenide Material Model

### Conduction Band Model

*Table 214 Position and orientation parameters of L-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
y	Y	Orientation of the y-axis	1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 1 0	$\langle hkl \rangle$
<b>L3</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 -0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 -1 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$
<b>L4</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	1 1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L5</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 -0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 -1 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 -1 -2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L6</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 1 -1	$\langle hkl \rangle$

## Chapter 17: Indium Gallium Arsenide Material Model

### Conduction Band Model

*Table 214 Position and orientation parameters of L-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
y	Y	Orientation of the y-axis	1 -1 -2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$
<b>L7</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 -0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 -1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$
<b>L8</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 -0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 -1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 1 0	$\langle hkl \rangle$

*Table 215 Position and orientation parameters of  $\Gamma$ -minimum of conduction band*

Parameter symbol	Parameter name	Description	Default	Unit
<b>G</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.0	$2\pi/a$
x	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$

## Chapter 17: Indium Gallium Arsenide Material Model

### Conduction Band Model

## Parameters

To change the default parameter values of the valley minima models, listed in the following tables, for each valleys listed in [Table 212](#), use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.conduction.C1.<valley>.<parameter> <value>
```

### Note:

By default, all  $X$ -minima have the same parameter values, and all  $L$ -minima have the same parameter values.

*Table 216 Parameters of X-valley model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Minima with respect to band edge	0.59	eV
$m_x$	$m_x$	Longitudinal effective mass	1.2099	$m_e$
$m_y$	$m_y$	Transverse effective mass	0.1929	$m_e$
$m_z$	$m_z$	Transverse effective mass	0.1929	$m_e$
$\alpha$	$a$	Valley nonparabolicity factor	0.65	—
$\Xi_u$	$\xi_u$	Uniaxial deformation potential	0.0	eV
$\Xi_d$	$\xi_d$	Dilatation deformation potential	0.0	eV
$\Xi'_u$	$\xi'_u$	Uniaxial mass deformation	0.0	eV

*Table 217 Parameters of L-valley model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Minima with respect to band edge	0.46	eV
$m_x$	$m_x$	Longitudinal effective mass	1.2322	$m_e$

## Chapter 17: Indium Gallium Arsenide Material Model

### Conduction Band Model

Table 217 Parameters of L-valley model (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$m_y$	my	Transverse effective mass	0.0614	$m_e$
$m_z$	mz	Transverse effective mass	0.0614	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.4265	—
$\Xi_u$	xi_u	Uniaxial deformation potential	0.0	eV
$\Xi_d$	xi_d	Dilatation deformation potential	0.0	eV
$\Xi'_u$	xi_u_prime	Uniaxial mass deformation	0.0	eV

Table 218 Parameters of  $\Gamma$ -valley model

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Minima with respect to band edge	0.0	eV
$m_x$	mx	Longitudinal effective mass	0.041	$m_e$
$m_y$	my	Transverse effective mass	0.041	$m_e$
$m_z$	mz	Transverse effective mass	0.041	$m_e$
$\alpha$	a	Valley nonparabolicity factor	1.7112	—
$\Xi_u$	xi_u	Uniaxial deformation potential	0.0	eV
$\Xi_d$	xi_d	Dilatation deformation potential	0.0	eV
$\Xi'_u$	xi_u_prime	Uniaxial mass deformation	0.0	eV

## Chapter 17: Indium Gallium Arsenide Material Model

### Conduction Band Model

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## X-Valley Scattering Mechanisms

The six X-minima define the set of scattering mechanisms listed in [Table 219](#). By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.conduction.C1.<valley>.<mechanism> ADD
```

```
MATERIAL In53Ga47As_fixed.conduction.C1.<valley>.<mechanism> REMOVE
```

*Table 219 Scattering mechanisms for X-minima*

Scattering mechanism	X1	X2	X3	X4	X5	X6
	Mechanism name					
Acoustic Phonon (elastic)	ac	ac	ac	ac	ac	ac
Polar Optical (intra)	pop	pop	pop	pop	pop	pop
Optical Phonon (inter)	opx2	opx1	opx1	opx1	opx1	opx1
Optical Phonon (inter)	opx3	opx3	opx2	opx3	opx3	opx3
Optical Phonon (inter)	opx4	opx4	opx4	opx2	opx4	opx4
Optical Phonon (inter)	opx5	opx5	opx5	opx5	opx2	opx5
Optical Phonon (inter)	opx6	opx6	opx6	opx6	opx6	opx2
Optical Phonon (inter)	opl1	opl1	opl1	opl1	opl1	opl1
Optical Phonon (inter)	opl2	opl2	opl2	opl2	opl2	opl2
Optical Phonon (inter)	opl3	opl3	opl3	opl3	opl3	opl3
Optical Phonon (inter)	opl4	opl4	opl4	opl4	opl4	opl4
Optical Phonon (inter)	opl5	opl5	opl5	opl5	opl5	opl5
Optical Phonon (inter)	opl6	opl6	opl6	opl6	opl6	opl6
Optical Phonon (inter)	opl7	opl7	opl7	opl7	opl7	opl7
Optical Phonon (inter)	opl8	opl8	opl8	opl8	opl8	opl8

## Chapter 17: Indium Gallium Arsenide Material Model

### Conduction Band Model

Table 219 Scattering mechanisms for X-minima (Continued)

Scattering mechanism	X1	X2	X3	X4	X5	X6
Mechanism name						
Optical Phonon (inter)	opg	opg	opg	opg	opg	opg
Ionized Impurity	II	II	II	II	II	II
Surface Roughness	SR	SR	SR	SR	SR	SR
Remote Coulomb	RC	RC	RC	RC	RC	RC

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each X-minimum, listed in [Table 219](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.conduction.C1.<valley>.<mechanism>.<parameter>
<value>
```

### Elastic Acoustic Phonon Scattering

[Table 220](#) lists the default parameter values of intravalley elastic acoustic phonon scattering.

Table 220 Parameters of elastic acoustic phonon scattering

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
		Mechanism name:	ac						
		Description	Default						
$\Delta_{ac}$	D	Acoustic deformation	5.424						eV
$v$	v	Velocity		3.45×10 <sup>3</sup>					m/s
$i$	final	Final minima	X1	X2	X3	X4	X5	X6	–

## Chapter 17: Indium Gallium Arsenide Material Model

Conduction Band Model

### Polar-Optical Phonon Scattering

[Table 221](#) lists the default parameter values of intravalley polar-optical phonon scattering.

*Table 221 Parameters of polar-optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
<b>Mechanism name:</b> pop									
<b>Description</b>									<b>Default</b>
$E_{op}$	E	Phonon energy							eV
$i$	final	Final minima	X1	X2	X3	X4	X5	X6	—

### Optical Phonon Scattering

[Table 222](#) to [Table 224](#) list the default parameter values of intervalley optical phonon scattering.

*Table 222 Parameters of intervalley X to X optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
<b>Mechanism name:</b> opx [1, 2, 3, 4, 5, 6]									
<b>Description</b>									<b>Default</b>
$E_{op}$	E	Phonon energy							eV
$D_{op}$	Cc	Coupling constant							eV/m
$i$	final	Final minima	X[1, 2, 3, 4, 5, 6]						—

*Table 223 Parameters of intervalley X to L optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
<b>Mechanism name:</b> opl[1, 2, 3, 4, 5, 6, 7, 8]									
<b>Description</b>									<b>Default</b>
$E_{op}$	E	Phonon energy							eV

## Chapter 17: Indium Gallium Arsenide Material Model

### Conduction Band Model

Table 223 Parameters of intervalley X to L optical phonon scattering (Continued)

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
		Mechanism name:	opl[1, 2, 3, 4, 5, 6, 7, 8]						
		Description	Default						
$D_{op}$	cc	Coupling constant							eV/m
$i$	final	Final minima							—

Table 224 Parameters of intervalley X to  $\Gamma$  optical phonon scattering

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
		Mechanism name:	opg						
		Description	Default						
$E_{op}$	E	Phonon energy							eV
$D_{op}$	cc	Coupling constant							eV/m
$i$	final	Final minima							—

## L-Valley Scattering Mechanisms

The eight L-minima define the set of scattering mechanisms listed in Table 225. By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.conduction.C1.<valley>.<mechanism> ADD
MATERIAL In53Ga47As_fixed.conduction.C1.<valley>.<mechanism> REMOVE
```

## Chapter 17: Indium Gallium Arsenide Material Model

### Conduction Band Model

Table 225 Scattering mechanisms for L-minima

Scattering mechanism	L1	L2	L3	L4	L5	L6	L7	L8
	Mechanism name							
Acoustic Phonon (elastic)	ac	ac	ac	ac	ac	ac	ac	ac
Polar Optical (intra)	pop	pop	pop	pop	pop	pop	pop	pop
Optical Phonon (intra)	opl	opl	opl	opl	opl	opl	opl	opl
Optical Phonon (inter)	opl2	opl1						
Optical Phonon (inter)	opl3	opl3	opl2	opl2	opl2	opl2	opl2	opl2
Optical Phonon (inter)	opl4	opl4	opl4	opl3	opl3	opl3	opl3	opl3
Optical Phonon (inter)	opl5	opl5	opl5	opl5	opl4	opl4	opl4	opl4
Optical Phonon (inter)	opl6	opl6	opl6	opl6	opl6	opl5	opl5	opl5
Optical Phonon (inter)	opl7	opl7	opl7	opl7	opl7	opl7	opl6	opl6
Optical Phonon (inter)	opl8	opl8	opl8	opl8	opl8	opl8	opl8	opl7
Optical Phonon (inter)	opx1	opx1	opx1	opx1	opx1	opx1	opx1	opx1
Optical Phonon (inter)	opx2	opx2	opx2	opx2	opx2	opx2	opx2	opx2
Optical Phonon (inter)	opx3	opx3	opx3	opx3	opx3	opx3	opx3	opx3
Optical Phonon (inter)	opx4	opx4	opx4	opx4	opx4	opx4	opx4	opx4
Optical Phonon (inter)	opx5	opx5	opx5	opx5	opx5	opx5	opx5	opx5
Optical Phonon (inter)	opx6	opx6	opx6	opx6	opx6	opx6	opx6	opx6
Optical Phonon (inter)	opg	opg	opg	opg	opg	opg	opg	opg
Ionized Impurity	II	II	II	II	II	II	II	II
Surface Roughness	SR	SR	SR	SR	SR	SR	SR	SR
Remote Coulomb	RC	RC	RC	RC	RC	RC	RC	RC

## Chapter 17: Indium Gallium Arsenide Material Model

Conduction Band Model

### Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each  $L$ -minimum, listed in [Table 225](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.conduction.C1.<valley>.<mechanism>.<parameter><value>
```

#### Inelastic Acoustic Phonon Scattering

[Table 226](#) lists the default parameter values of intravalley inelastic *longitudinal* acoustic phonon scattering.

*Table 226 Parameters of inelastic longitudinal acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	ac								
Description											Default
$\Delta_{ac}$	D	Acoustic deformation	5.424								eV
$v$	v	Velocity	3.45×10 <sup>3</sup>								m/s
$i$	final	Final minima	L1	L2	L3	L4	L5	L6	L7	L8	—

#### Polar-Optical Phonon Scattering

[Table 227](#) lists the default parameter values of intravalley polar-optical phonon scattering.

*Table 227 Parameters of polar-optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	pop								
Description											Default
$E_{op}$	E	Phonon energy	35.0×10 <sup>-3</sup>								eV
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]								—

## Chapter 17: Indium Gallium Arsenide Material Model

Conduction Band Model

### Optical Phonon Scattering

[Table 228](#) to [Table 231](#) list the default parameter values of intravalley and intervalley optical phonon scattering.

*Table 228 Parameters of intravalley optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opl[1, 2, 3, 4, 5, 6, 7, 8]								
		Description	Default								
$E_{op}$	E	Phonon energy									eV
$D_{op}$	Cc	Coupling constant									eV/m
$i$	final	Final minima									—

*Table 229 Parameters of intervalley L to L optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opl[1, 2, 3, 4, 5, 6, 7, 8]								
		Description	Default								
$E_{op}$	E	Phonon energy									eV
$D_{op}$	Cc	Coupling constant									eV/m
$i$	final	Final minima									—

*Table 230 Parameters of intervalley L to X optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opx[1, 2, 3, 4, 5, 6]								
		Description	Default								
$E_{op}$	E	Phonon energy									eV

## Chapter 17: Indium Gallium Arsenide Material Model

Conduction Band Model

Table 230 Parameters of intervalley L to X optical phonon scattering (Continued)

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opx[1, 2, 3, 4, 5, 6]								
		Description	Default								
$D_{op}$	Cc	Coupling constant									eV/m
$i$	final	Final minima									-

Table 231 Parameters of intervalley L to  $\Gamma$  optical phonon scattering

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opg								
		Description	Default								
$E_{op}$	E	Phonon energy									eV
$D_{op}$	Cc	Coupling constant									eV/m
$i$	final	Final minima									-

## $\Gamma$ -Valley Scattering Mechanisms

The  $\Gamma$ -minimum defines the set of scattering mechanisms listed in Table 232. By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.conduction.C2.G.<mechanism> ADD
```

```
MATERIAL In53Ga47As_fixed.conduction.C2.G.<mechanism> REMOVE
```

**Chapter 17: Indium Gallium Arsenide Material Model**

## Conduction Band Model

*Table 232 Scattering mechanisms for  $\Gamma$ -minimum*

Scattering mechanism	Mechanism name
Acoustic Phonon (elastic)	ac
Polar Optical (intra)	pop
Optical Phonon (inter)	opl1
Optical Phonon (inter)	opl2
Optical Phonon (inter)	opl3
Optical Phonon (inter)	opl4
Optical Phonon (inter)	opl5
Optical Phonon (inter)	opl6
Optical Phonon (inter)	opl7
Optical Phonon (inter)	opl8
Optical Phonon (inter)	opx1
Optical Phonon (inter)	opx2
Optical Phonon (inter)	opx3
Optical Phonon (inter)	opx4
Optical Phonon (inter)	opx5
Optical Phonon (inter)	opx6
Ionized Impurity	II
Surface Roughness	SR
Remote Coulomb	RC

## Chapter 17: Indium Gallium Arsenide Material Model

Conduction Band Model

### Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for the  $\Gamma$ -minimum, listed in [Table 232](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.conduction.C2.G.<mechanism>. <parameter> <value>
```

#### Inelastic Acoustic Phonon Scattering

[Table 233](#) lists the default parameter values of intravalley inelastic *longitudinal* acoustic phonon scattering.

*Table 233 Parameters of inelastic longitudinal acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	ac	
		Description	Default	
$\Delta_{ac}$	D	Acoustic deformation	5.424	eV
$v$	v	Velocity	$3.45 \times 10^3$	m/s
$i$	final	Final minima	G	—

#### Polar-Optical Phonon Scattering

[Table 234](#) lists the default parameter values of intravalley polar-optical phonon scattering.

*Table 234 Parameters of polar-optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	pop	
		Description	Default	
$E_{op}$	E	Phonon energy	$35.0 \times 10^{-3}$	eV
$i$	final	Final minima	G	—

## Chapter 17: Indium Gallium Arsenide Material Model

### Conduction Band Model

#### Optical Phonon Scattering

[Table 235](#) and [Table 236](#) list the default parameter values of intervalley optical phonon scattering.

*Table 235 Parameters of intervalley  $\Gamma$  to L optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
<b>Mechanism name:</b> opl[1, 2, 3, 4, 5, 6, 7, 8]				
<b>Description</b>				<b>Default</b>
$E_{op}$	E	Phonon energy	$19.9128 \times 10^{-3}$	eV
$D_{op}$	Cc	Coupling constant	$5.4302 \times 10^{10}$	eV/m
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]	-

*Table 236 Parameters of intervalley  $\Gamma$  to X optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
<b>Mechanism name:</b> opx[1, 2, 3, 4, 5, 6]				
<b>Description</b>				<b>Default</b>
$E_{op}$	E	Phonon energy	$21.2134 \times 10^{-3}$	eV
$D_{op}$	Cc	Coupling constant	$25.0 \times 10^{10}$	eV/m
$i$	final	Final minima	X[1, 2, 3, 4, 5, 6]	-

---

## Ionized Impurity Scattering

Ionized impurity scattering is defined for each valley in a conduction band and is treated as an intravalley process by default, so that the final valley after scattering is the same as the initial valley.

*Table 237 Parameters of ionized impurity scattering*

Parameter symbol	Parameter name	Valley name:	All valleys	Unit
		<b>Mechanism name:</b>	II	
		<b>Description</b>	<b>Default</b>	
<i>i</i>	final	Final minimum	Same as initial minimum	–

## Ionized Impurity Empirical Rate Factor

The ionized impurity scattering model includes a scaling factor for the empirical correction of the calculated scattering rate as a function of doping density.

To redefine the default empirical factor, use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.conduction.IIfac N <Nvalue> [<Nvalue2>] <rule>
<value>
```

Here, **IIfac** is a piecewise interpolation parameter that defines a correction factor **<value>** for a value **<Nvalue>** of the doping concentration **N**. The interpolation model used to return values between specified densities is given by **<rule>**, which might require an upper bound of the density [**<Nvalue2>**]. For a description of the interpolation parameter type, see [Interpolation Methods on page 301](#).

By default, the empirical correction for ionized impurity is 1.0. However, for electrons in  $\text{In}_{53}\text{Ga}_{47}\text{As}$ , a non-unity default value is provided to best match experimental low-field concentration-dependent mobility.

---

## Surface Roughness Scattering

[Table 238](#) lists the default parameter values of surface roughness scattering. These parameters apply to all valleys and to all equivalent surface orientations.

*Table 238 Parameters of surface roughness scattering*

<b>Parameter symbol</b>	<b>Parameter name</b>	<b>Mechanism name:</b>	<b>SR</b>		<b>Unit</b>
		<b>Description</b>	<b>Default</b>		
$\Delta$	rms	RMS amplitude	1.2	1.2	nm
$L_c$	l	Correlation length	1.0	1.0	nm
$\langle hkl \rangle$	orient	Surface orientation	(001)	(110)	–
$i$	carrier	Carrier type	electrons	electrons	–

---

## Remote Coulomb Scattering

[Table 239](#) lists the default parameter values of remote Coulomb scattering, which is treated as an intravalley process. These parameters apply to all valleys.

*Table 239 Parameters of remote Coulomb scattering*

<b>Parameter symbol</b>	<b>Parameter name</b>	<b>Mechanism name:</b>	<b>RC</b>		<b>Unit</b>
		<b>Description</b>	<b>Default</b>		
$z_d$	zd	Depth of charge centroid	1.5		nm
$E_0$	E0	Minimum energy for tabulating rate	0		eV
$N_0$	N0	Minimum screening density	$5 \times 10^{15}$		$\text{cm}^{-3}$
$i$	final	Final minimum	Same as initial minimum		–

---

To define the interface charge density for remote Coulomb scattering, follow the descriptions in [Defining Interface Models on page 217](#). By default, no interface charge is applied.

## Chapter 17: Indium Gallium Arsenide Material Model

### Valence Band Model

## Valence Band Model

This section describes the valence band model.

### Band Edge Parameters

To change the default parameter values of the valence band container model, listed in [Table 240](#), use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.valence.<parameter> <value>
```

*Table 240 Parameters of valence band container model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Valence band energy with respect to vacuum	5.24	eV
$m_{dg_x}$	$dgx$	Hole density gradient effective x-mass	0.5	$m_e$
$m_{dg_y}$	$dgy$	Hole density gradient effective y-mass	0.5	$m_e$
$m_{dg_z}$	$dgz$	Hole density gradient effective z-mass	0.5	$m_e$
<b>k-p band structure model parameters</b>				
$L$	$L-kp$	Valence band parameter	0.0	$\hbar^2/2m$
$M$	$M-kp$	Valence band parameter	0.0	$\hbar^2/2m$
$N$	$N-kp$	Valence band parameter	0.0	$\hbar^2/2m$
$l$	$l-defpot$	Valence deformation potential	0.0	eV
$m$	$m-defpot$	Valence deformation potential	0.0	eV
$n$	$n-defpot$	Valence deformation potential	0.0	eV
$\Delta_{sso}$	$dsso$	Spin-orbit split energy	0.0	eV

## Chapter 17: Indium Gallium Arsenide Material Model

### Valence Band Model

To change the default parameter values of the valence bands in the container model, listed in [Table 241](#), use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.valence.<band>.<parameter> <value>
```

*Table 241 Parameters of valence band model*

Parameter symbol	Parameter name	Description	Default	Unit
<b>Heavy hole (HH) band</b>				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.0	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	6kp	—
<b>Light hole (LH) band</b>				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.0	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	6kp	—
<b>Spin split-off (SSO) band</b>				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.044	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	6kp	—

## Mobility Models

The valence band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models together with some phenomenological enhancement factors.

### Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 242](#), use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.valence.constant.<parameter> <value>
```

## Chapter 17: Indium Gallium Arsenide Material Model

### Valence Band Model

Table 242 Parameters of constant mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	320	cm <sup>2</sup> /Vs
$\zeta$	zeta	Fitting parameter	1.59	—

## Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 243](#), use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.valence.Arora.<parameter> <value>
```

Table 243 Parameters of Arora mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min}$	mumin	Minimum mobility	54.3	cm <sup>2</sup> /Vs
$\mu_{\max}$	mumax	Maximum mobility	320	cm <sup>2</sup> /Vs
$N_0$	n0	Reference concentration	$2.35 \times 10^{17}$	cm <sup>-3</sup>
$\alpha$	alpha	Fitting parameter	0.88	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.33	—
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

## Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 244](#), use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.valence.Masetti.<parameter> <value>
```

## Chapter 17: Indium Gallium Arsenide Material Model

### Valence Band Model

*Table 244 Parameters of Masetti mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min 1}$	mumin1	Minimum mobility	75.0	cm <sup>2</sup> /Vs
$\mu_{\min 2}$	mumin2	Minimum mobility	75.0	cm <sup>2</sup> /Vs
$\mu_{\max}$	mumax	Maximum mobility	320	cm <sup>2</sup> /Vs
$\mu_1$	mul	Maximum mobility	1.0	cm <sup>2</sup> /Vs
$C_r$	cr	Reference concentration	$1.0 \times 10^{18}$	cm <sup>-3</sup>
$C_s$	cs	Reference solid solubility concentration	1.0	cm <sup>-3</sup>
$p_c$	pc	Reference concentration	0.0	cm <sup>-3</sup>
$\alpha$	alpha	Fitting parameter	2.37	—
$\beta$	beta	Fitting parameter	2.0	—
$\zeta$	zeta	Fitting parameter	2.2	—

## Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 245](#), use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.valence.Yamaguchi.<parameter> <value>
```

*Table 245 Parameters of Yamaguchi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

## Chapter 17: Indium Gallium Arsenide Material Model

### Valence Band Model

## Perpendicular Field: Lombardi Mobility Model

To change the default parameter values of the Lombardi mobility model, listed in [Table 246](#), use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.valence.Lombardi.<parameter> <value>
```

*Table 246 Parameters of Lombardi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
A	a	Fitting parameter	2.0	—
B	b	Fitting parameter	$9.925 \times 10^6$	cm/s
C	c	Fitting parameter	$2.947 \times 10^3$	$\text{cm}^{5/3} \text{V}^{-2/3} \text{s}^{-1}$
$\alpha$	alpha	Fitting parameter	0.0	$\text{cm}^3$
$\delta$	delta	Fitting parameter	$2.0546 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$2.0546 \times 10^{30}$	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	1.0	—
$\lambda$	lambda	Fitting parameter	0.0317	—
v	nu	Fitting parameter	1.0	—
$N_0$	n0	Fitting parameter	1.0	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	1.0	$\text{cm}^{-3}$
$l_{\text{crit}}$	lcrit	Critical length	$1 \times 10^{-6}$	cm

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in [Table 247](#), use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.valence.Caughey.<parameter> <value>
```

## Chapter 17: Indium Gallium Arsenide Material Model

### Valence Band Model

Table 247 Parameters of Caughey–Thomas mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$4.5 \times 10^6$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	0.52	—
$\beta_0$	beta0	Fitting parameter	1.213	—
$\beta_{\text{exp}}$	bexp	Fitting parameter	0.17	—
$\alpha$	alpha	Fitting parameter	0.0	—

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 248](#). To change the default mobility model, use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.valence.mobility.<model> <value>
```

Table 248 Parameters of default mobility model

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley valence band model consists of the valley minima listed in [Table 249](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.valence.<band>.<valley> REMOVE
```

### Note:

The valence band analytic valley approximation is used only as a way to define density-of-states for drift diffusion simulations and to define the valley minima in response to stress.

## Chapter 17: Indium Gallium Arsenide Material Model

### Valence Band Model

Table 249 Names of valence band minima

Valence band minimum	Band name	Valley name
Heavy hole	HH	vhh
Light hole	LH	vlh
Spin split-off	SSO	vsso

## Position and Orientation

The position and orientation of the HH, LH, and SSO valley minima are identical. [Table 250](#) shows the default values. To change the default values, use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.valence.<band>.<valley>.min.<parameter> <value>
```

Table 250 Position and orientation parameters of HH, LH, and SSO valley minima

Parameter symbol	Parameter name	Description	Default	Unit
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.0	$2\pi/a$
x	x	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
y	y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
z	z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$

## Parameters

To change the valley minima model parameters, listed in [Table 251](#), for each valley listed in [Table 249](#), use the following input file syntax:

```
MATERIAL In53Ga47As_fixed.valence.<band>.<valley>.<parameter> <value>
```

Table 251 Parameters of valence band minima

Parameter symbol	Parameter name	Description	Default	Unit
<b>Heavy hole (HH) band</b>				
E	E	Minima with respect to band edge	0.0	eV

## Chapter 17: Indium Gallium Arsenide Material Model

### Valence Band Model

Table 251 Parameters of valence band minima (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$m_x$	mx	Longitudinal effective mass	0.45	$m_e$
$m_y$	my	Transverse effective mass	0.45	$m_e$
$m_z$	mz	Transverse effective mass	0.45	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	0.0	eV
<b>Light hole (LH) band</b>				
$E$	E	Minima with respect to band edge	0.0	eV
$m_x$	mx	Longitudinal effective mass	0.052	$m_e$
$m_y$	my	Transverse effective mass	0.052	$m_e$
$m_z$	mz	Transverse effective mass	0.052	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	0.0	eV
<b>Spin split-off (SSO) band</b>				
$E$	E	Minima with respect to band edge	0.32961	eV
$m_x$	mx	Longitudinal effective mass	0.15	$m_e$
$m_y$	my	Transverse effective mass	0.15	$m_e$
$m_z$	mz	Transverse effective mass	0.15	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	0.0	eV

## **Heavy-Hole Band Scattering Mechanisms**

There are no heavy-hole band scattering mechanisms defined in the current version of Garand.

---

## **Light-Hole Band Scattering Mechanisms**

There are no light-hole band scattering mechanisms defined in the current version of Garand.

---

## **Spin Split-Off Band Scattering Mechanisms**

There are no spin split-off band scattering mechanisms defined in the current version of Garand.

---

## **Simulation Results**

This section presents various simulation results for the  $\text{In}_{53}\text{Ga}_{47}\text{As}$  material model.

---

## **Velocity-Field Characteristics**

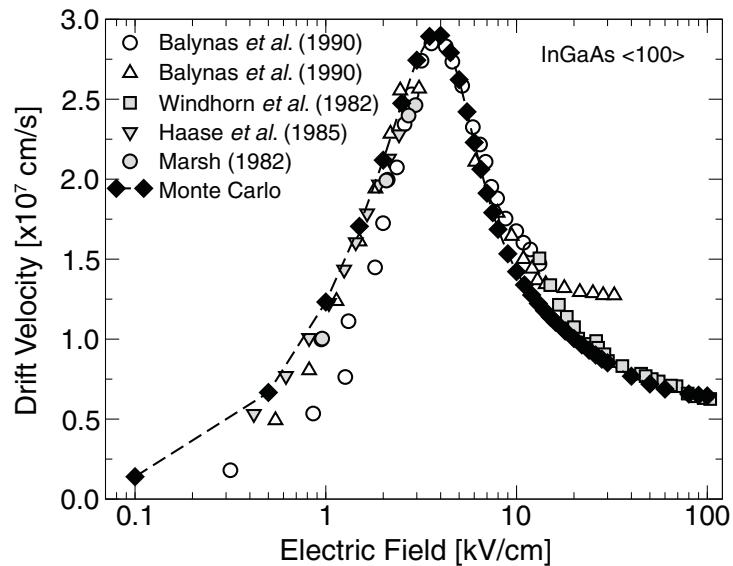
The velocity-field characteristics of InGaAs material have been calibrated to experimental data for InGaAs (with fractions of  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ ) at 300 K [1][2][3][4].

Figure 49 shows the resultant calibration with experimental data.

## Chapter 17: Indium Gallium Arsenide Material Model

### Simulation Results

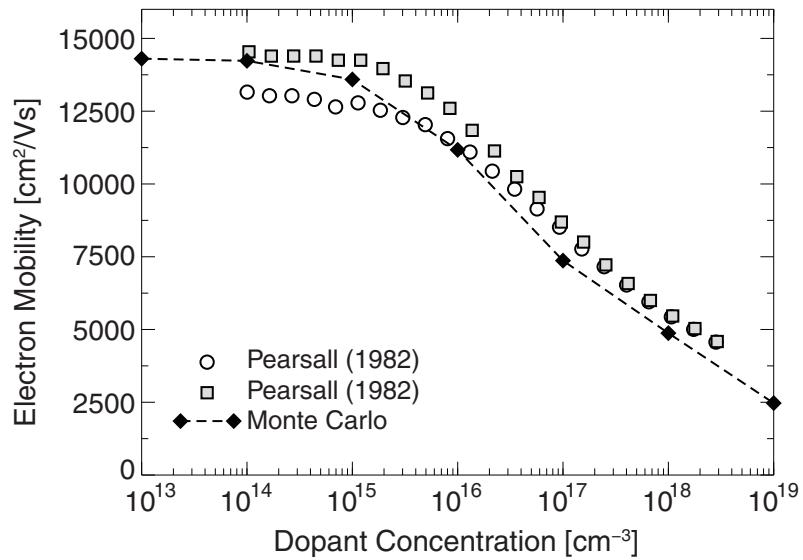
Figure 49 Calibrated velocity-field characteristics for InGaAs material



## Low-Field Concentration-Dependent Mobility

Figure 50 shows the simulated low-field electron mobility in InGaAs (with fractions of  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ ) at 300 K in comparison with experimental data from [5].

Figure 50 Doping-dependent low-field electron mobility in InGaAs compared to experimental measurements [5]



## References

- [1] V. Balynas *et al.*, "Time-Resolved, Hot-Electron Conductivity Measurement Using an Electro-Optic Sampling Technique," *Applied Physics A: Materials Science and Processing*, vol. 51, no. 4, pp. 357–360, 1990.
- [2] T. H. Windhorn, L. W. Cook, and G. E. Stillman, "Temperature Dependent Electron Velocity-Field Characteristics for  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$  at High Electric Fields," *Journal of Electronic Materials*, vol. 11, no. 6, pp. 1065–1082, 1982.
- [3] M. A. Haase *et al.*, "Subthreshold electron velocity-field characteristics of GaAs and  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ ," *Journal of Applied Physics*, vol. 57, no. 6, pp. 2295–2298, 1985.
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- [5] T. P. Pearsall (ed.), *GaInAsP Alloy Semiconductors*, John Wiley & Sons, 1982.

## Indium Aluminum Arsenide Material Model

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*This chapter describes the  $In_{52}Al_{48}As$  material model.*

---

### Bulk Material Model

This section describes the bulk material model for  $In_{52}Al_{48}As$ .

---

#### Parameters of Bulk Material Model

To change the default parameter values listed in [Table 252](#), use the following input file syntax:

```
MATERIAL In52Al48As_fixed.<parameter> <value>
```

*Table 252 Bulk material model parameters*

Parameter symbol	Parameter name	Description	Default	Unit
<b>Crystal lattice and orientation in simulation domain</b>				
$ a $	a	Magnitude of lattice vector a	5.8676	Å
$ b $	b	Magnitude of lattice vector b	5.8676	Å
$ c $	c	Magnitude of lattice vector c	5.8676	Å
$\alpha$	alpha	Angle between b and c	90	degree
$\beta$	beta	Angle between c and a	90	degree
$\gamma$	gamma	Angle between a and b	90	degree

## Chapter 18: Indium Aluminum Arsenide Material Model

### Conduction Band Model

Table 252 Bulk material model parameters (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$\langle hkl \rangle_x$	x	Orientation in the x-direction	1 0 0	—
$\langle hkl \rangle_z$	z	Orientation in the z-direction	0 0 1	—
<b>Bulk electrical and mechanical properties</b>				
$\kappa$	permittivity	Relative dielectric constant	12.7068	—
$\kappa_\infty$	k_inf	High-frequency permittivity	10.5468	—
$\rho$	density	Mass density	4.7584	g/cm <sup>3</sup>
$C_{11}$	C11	Elastic stiffness matrix element	168.3	GPa
$C_{12}$	C12	Elastic stiffness matrix element	66.8	GPa
$C_{44}$	C44	Elastic stiffness matrix element	79.9	GPa

## Band-to-Band Tunneling Parameters

To change the default parameter values for the Kane model, listed in Table 253, use the following input file syntax:

```
MATERIAL In52Al48As_fixed.BTBT.<parameter> <value>
```

Table 253 Band-to-band tunneling parameters

Parameter symbol	Parameter name	Description	Default	Unit
$D_{TA}$	DTA	Acoustic phonon deformation potential	0.0	eV
$\epsilon_{TA}$	epsilonTA	Acoustic phonon energy	0.0	eV

## Conduction Band Model

This section describes the conduction band model.

## Chapter 18: Indium Aluminum Arsenide Material Model

### Conduction Band Model

---

## Band Edge Parameters

To change the default parameter values of the conduction band container model, listed in [Table 254](#), use the following input file syntax:

```
MATERIAL In52Al48As_fixed.conduction.<parameter> <value>
```

*Table 254 Parameters of conduction band container model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Conduction band energy with respect to vacuum	4.228	eV
$m_{dg_x}$	dgx	Electron density gradient effective x-mass	0.3	$m_e$
$m_{dg_y}$	dgy	Electron density gradient effective y-mass	0.3	$m_e$
$m_{dg_z}$	dgz	Electron density gradient effective z-mass	0.3	$m_e$

To change the default parameter values of the conduction bands in the container model, listed in [Table 255](#), use the following input file syntax:

```
MATERIAL In52Al48As_fixed.conduction.<band>.<parameter> <value>
```

*Table 255 Parameters of conduction band model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Conduction band energy with respect to container energy	0.0	eV
$model$	model	Model used for transport in this band	ema	—

---

## Mobility Models

The conduction band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models.

## Chapter 18: Indium Aluminum Arsenide Material Model

### Conduction Band Model

## Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 256](#), use the following input file syntax:

```
MATERIAL In52Al48As_fixed.conduction.constant.<parameter> <value>
```

*Table 256 Parameters of constant mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	12550	$\text{cm}^2/\text{Vs}$
$\zeta$	zeta	Fitting parameter	2.5	—

## Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 257](#), use the following input file syntax:

```
MATERIAL In52Al48As_fixed.conduction.Arora.<parameter> <value>
```

*Table 257 Parameters of Arora mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min}$	mumin	Minimum mobility	88.0	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	umax	Maximum mobility	12550	$\text{cm}^2/\text{Vs}$
$N_0$	n0	Reference concentration	$1.25 \times 10^{17}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.88	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.33	—
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

## Chapter 18: Indium Aluminum Arsenide Material Model

Conduction Band Model

### Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 258](#), use the following input file syntax:

```
MATERIAL In52Al48As_fixed.conduction.Masetti.<parameter> <value>
```

*Table 258 Parameters of Masetti mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min 1}$	mumin1	Minimum mobility	100.0	$\text{cm}^2/\text{Vs}$
$\mu_{\min 2}$	mumin2	Minimum mobility	100.0	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	12550	$\text{cm}^2/\text{Vs}$
$\mu_1$	mul	Maximum mobility	1	$\text{cm}^2/\text{Vs}$
$C_r$	cr	Reference concentration	$3.2 \times 10^{17}$	$\text{cm}^{-3}$
$C_s$	cs	Reference solid solubility concentration	0.0	$\text{cm}^{-3}$
$p_c$	pc	Reference concentration	0.0	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.5	—
$\beta$	beta	Fitting parameter	2.0	—
$\zeta$	zeta	Fitting parameter	2.5	—

### Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 259](#), use the following input file syntax:

## Chapter 18: Indium Aluminum Arsenide Material Model

### Conduction Band Model

```
MATERIAL In52Al48As_fixed.conduction.Yamaguchi.<parameter> <value>
```

Table 259 Parameters of Yamaguchi mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

## Perpendicular Field: Lombardi Mobility Model

To change the default parameter values of the Lombardi mobility model, listed in [Table 260](#), use the following input file syntax:

```
MATERIAL In52Al48As_fixed.conduction.Lombardi.<parameter> <value>
```

Table 260 Parameters of Lombardi mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$A$	a	Fitting parameter	2.0	—
$B$	b	Fitting parameter	$4.75 \times 10^7$	cm/s
$C$	c	Fitting parameter	$5.80 \times 10^2$	$\text{cm}^{5/3} \text{V}^{-2/3} \text{s}^{-1}$
$\alpha$	alpha	Fitting parameter	0.0	$\text{cm}^3$
$\delta$	delta	Fitting parameter	$5.82 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$5.82 \times 10^{30}$	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	1.0	—
$\lambda$	lambda	Fitting parameter	0.125	—
$\nu$	nu	Fitting parameter	1.0	—
$N_0$	n0	Fitting parameter	1.0	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	1.0	$\text{cm}^{-3}$

## Chapter 18: Indium Aluminum Arsenide Material Model

### Conduction Band Model

Table 260 Parameters of Lombardi mobility model (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$l_{\text{crit}}$	lcrit	Critical length	$1 \times 10^{-6}$	cm

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in [Table 261](#), use the following input file syntax:

```
MATERIAL In52Al48As_fixed.conduction.Caughey.<parameter> <value>
```

Table 261 Parameters of Caughey–Thomas mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$8.9 \times 10^6$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	0.87	—
$\beta_0$	beta0	Fitting parameter	1.109	—
$\beta_{\text{exp}}$	bexp	Fitting parameter	0.66	—
$\alpha$	alpha	Fitting parameter	0.0	—

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 262](#). To change the default mobility model, use the following input file syntax:

```
MATERIAL In52Al48As_fixed.conduction.mobility.<model> <value>
```

## Chapter 18: Indium Aluminum Arsenide Material Model

### Conduction Band Model

Table 262 Parameters of default mobility model

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley conduction band model consists of the valley minima listed in [Table 263](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL In52Al48As_fixed.conduction.<band>.<valley> REMOVE
```

Table 263 Names of conduction band Cf1 minima

Conduction band minimum	Valley name
X	X1, X2, X3, X4, X5, X6
L	L1, L2, L3, L4, L5, L6, L7, L8
$\Gamma$	G

## Position and Orientation

Valley minima differ in their position and orientation, the default values of which are presented in [Table 264](#), [Table 265](#), and [Table 266](#).

To change default values, use the following input file syntax:

```
MATERIAL In52Al48As_fixed.conduction.C1.<valley>.min.<parameter> <value>
```

Table 264 Position and orientation parameters of X-minima of conduction band

Parameter symbol	Parameter name	Description	Default	Unit
<b>X1</b>				
$k_0$	pos	Position within the Brillouin zone	1.0 0.0 0.0	$2\pi/a$

## Chapter 18: Indium Aluminum Arsenide Material Model

### Conduction Band Model

*Table 264 Position and orientation parameters of X-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$x$	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X2</b>				
$k_0$	pos	Position within the Brillouin zone	-1.0 0.0 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X3</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 1.0 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	0 1 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X4</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 -1.0 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	0 1 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X5</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 1.0	$2\pi/a$

## Chapter 18: Indium Aluminum Arsenide Material Model

### Conduction Band Model

*Table 264 Position and orientation parameters of X-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$x$	X	Orientation of the x-axis	0 0 1	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 -1 0	$\langle hkl \rangle$
<b>X6</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 -1.0	$2\pi/a$
$x$	X	Orientation of the x-axis	0 0 1	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 -1 0	$\langle hkl \rangle$

*Table 265 Position and orientation parameters of L-minima of conduction band*

Parameter symbol	Parameter name	Description	Default	Unit
<b>L1</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 0.5 0.5	$2\pi/a$
$x$	X	Orientation of the x-axis	1 1 1	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 -1 2	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L2</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 0.5 0.5	$2\pi/a$
$x$	X	Orientation of the x-axis	-1 1 1	$\langle hkl \rangle$

## Chapter 18: Indium Aluminum Arsenide Material Model

### Conduction Band Model

*Table 265 Position and orientation parameters of L-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
y	Y	Orientation of the y-axis	1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 1 0	$\langle hkl \rangle$
<b>L3</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 -0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 -1 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$
<b>L4</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	1 1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L5</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 -0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 -1 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 -1 -2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L6</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 1 -1	$\langle hkl \rangle$

## Chapter 18: Indium Aluminum Arsenide Material Model

### Conduction Band Model

Table 265 Position and orientation parameters of L-minima of conduction band (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
y	Y	Orientation of the y-axis	1 -1 -2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$
<b>L7</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 -0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 -1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$
<b>L8</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 -0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 -1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 1 0	$\langle hkl \rangle$

Table 266 Position and orientation parameters of  $\Gamma$ -minimum of conduction band

Parameter symbol	Parameter name	Description	Default	Unit
<b>G</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.0	$2\pi/a$
x	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$

## Chapter 18: Indium Aluminum Arsenide Material Model

### Conduction Band Model

## Parameters

To change the default parameter values of the valley minima models, listed in the following tables, for each valley listed in [Table 263](#), use the following input file syntax:

```
MATERIAL In52Al48As_fixed.conduction.C1.<valley>.<parameter> <value>
```

### Note:

By default, all  $X$ -minima have the same parameter values, and all  $L$ -minima have the same parameter values.

*Table 267 Parameters of  $X$ -valley model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Minima with respect to band edge	0.2908	eV
$m_x$	$m_x$	Longitudinal effective mass	1.0532	$m_e$
$m_y$	$m_y$	Transverse effective mass	0.1888	$m_e$
$m_z$	$m_z$	Transverse effective mass	0.1888	$m_e$
$\alpha$	$a$	Valley nonparabolicity factor	0.6382	—
$\Xi_u$	$\xi_{u\text{--}}$	Uniaxial deformation potential	0.0	eV
$\Xi_d$	$\xi_{d\text{--}}$	Dilatation deformation potential	0.0	eV
$\Xi'_u$	$\xi'_{u\text{--}}$	Uniaxial mass deformation	0.0	eV

*Table 268 Parameters of  $L$ -valley model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Minima with respect to band edge	0.2404	eV
$m_x$	$m_x$	Longitudinal effective mass	0.9664	$m_e$

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### Conduction Band Model

Table 268 Parameters of  $L$ -valley model (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$m_y$	my	Transverse effective mass	0.098	$m_e$
$m_z$	mz	Transverse effective mass	0.098	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.45	—
$\Xi_u$	xi_u	Uniaxial deformation potential	0.0	eV
$\Xi_d$	xi_d	Dilatation deformation potential	0.0	eV
$\Xi'_u$	xi_u_prime	Uniaxial mass deformation	0.0	eV

Table 269 Parameters of  $\Gamma$ -valley model

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Minima with respect to band edge	0.0	eV
$m_x$	mx	Longitudinal effective mass	0.0733	$m_e$
$m_y$	my	Transverse effective mass	0.0733	$m_e$
$m_z$	mz	Transverse effective mass	0.0733	$m_e$
$\alpha$	a	Valley nonparabolicity factor	1.672	—
$\Xi_u$	xi_u	Uniaxial deformation potential	0.0	eV
$\Xi_d$	xi_d	Dilatation deformation potential	0.0	eV
$\Xi'_u$	xi_u_prime	Uniaxial mass deformation	0.0	eV

## Chapter 18: Indium Aluminum Arsenide Material Model

### Conduction Band Model

---

## X-Valley Scattering Mechanisms

The six *X*-minima define the set of scattering mechanisms listed in [Table 270](#). By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL In52Al48As_fixed.conduction.C1.<valley>.<mechanism> ADD
```

```
MATERIAL In52Al48As_fixed.conduction.C1.<valley>.<mechanism> REMOVE
```

*Table 270 Scattering mechanisms for X-minima*

Scattering mechanism	X1	X2	X3	X4	X5	X6
	Mechanism name					
Acoustic Phonon (elastic)	ac	ac	ac	ac	ac	ac
Polar Optical (intra)	pop	pop	pop	pop	pop	pop
Optical Phonon (inter)	opx1	opx1	opx1	opx1	opx1	opx1
Optical Phonon (inter)	opx2	opx2	opx2	opx2	opx2	opx2
Optical Phonon (inter)	opx3	opx3	opx3	opx3	opx3	opx3
Optical Phonon (inter)	opx4	opx4	opx4	opx4	opx4	opx4
Optical Phonon (inter)	opx5	opx5	opx5	opx5	opx5	opx5
Optical Phonon (inter)	opx6	opx6	opx6	opx6	opx6	opx6
Optical Phonon (inter)	opl1	opl1	opl1	opl1	opl1	opl1
Optical Phonon (inter)	opl2	opl2	opl2	opl2	opl2	opl2
Optical Phonon (inter)	opl3	opl3	opl3	opl3	opl3	opl3
Optical Phonon (inter)	opl4	opl4	opl4	opl4	opl4	opl4
Optical Phonon (inter)	opl5	opl5	opl5	opl5	opl5	opl5
Optical Phonon (inter)	opl6	opl6	opl6	opl6	opl6	opl6
Optical Phonon (inter)	opl7	opl7	opl7	opl7	opl7	opl7

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### Conduction Band Model

*Table 270 Scattering mechanisms for X-minima (Continued)*

Scattering mechanism	X1	X2	X3	X4	X5	X6
<b>Mechanism name</b>						
Optical Phonon (inter)	opl8	opl8	opl8	opl8	opl8	opl8
Optical Phonon (inter)	opg	opg	opg	opg	opg	opg
Ionized Impurity	II	II	II	II	II	II
Surface Roughness	SR	SR	SR	SR	SR	SR
Remote Coulomb	RC	RC	RC	RC	RC	RC

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each *X*-minimum, listed in [Table 270](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL In52Al48As_fixed.conduction.C1.<valley>.<mechanism>.<parameter>
<value>
```

### Elastic Acoustic Phonon Scattering

[Table 271](#) lists the default parameter values of intravalley elastic acoustic phonon scattering.

*Table 271 Parameters of elastic acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
		<b>Mechanism name: ac</b>							
		<b>Description</b>							
$\Delta_{ac}$	D	Acoustic deformation	6.376						eV
$v$	v	Velocity		3.81×10 <sup>3</sup>					m/s
$i$	final	Final minima	X1	X2	X3	X4	X5	X6	–

## Chapter 18: Indium Aluminum Arsenide Material Model

Conduction Band Model

### Polar-Optical Phonon Scattering

[Table 272](#) lists the default parameter values of intravalley polar-optical phonon scattering.

*Table 272 Parameters of polar-optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit		
		Mechanism name:	pop								
		Description	Default								
$E_{op}$	E	Phonon energy							eV		
$i$	final	Final minima	X1	X2	X3	X4	X5	X6	—		

### Optical Phonon Scattering

[Table 273](#) to [Table 275](#) list the default parameter values of intervalley optical phonon scattering.

*Table 273 Parameters of intervalley X to X optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit		
		Mechanism name:	opx [1, 2, 3, 4, 5, 6]								
		Description	Default								
$E_{op}$	E	Phonon energy							eV		
$D_{op}$	Cc	Coupling constant							eV/m		
$i$	final	Final minima							—		

## Chapter 18: Indium Aluminum Arsenide Material Model

Conduction Band Model

Table 274 Parameters of intervalley X to L optical phonon scattering

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
Mechanism name: opl[1, 2, 3, 4, 5, 6, 7, 8]									
		Description	Default						
$E_{op}$	E	Phonon energy	$20.2292 \times 10^{-3}$						eV
$D_{op}$	cc	Coupling constant	$6.0892 \times 10^{10}$						eV/m
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]						—

Table 275 Parameters of intervalley X to  $\Gamma$  optical phonon scattering

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
Mechanism name: opg									
		Description	Default						
$E_{op}$	E	Phonon energy	$22.0332 \times 10^{-3}$						eV
$D_{op}$	cc	Coupling constant	$6.806 \times 10^{10}$						eV/m
$i$	final	Final minima	G						—

## L-Valley Scattering Mechanisms

The eight L-minima define the set of scattering mechanisms listed in Table 276. By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL In52Al48As_fixed.conduction.C1.<valley>.<mechanism> ADD
MATERIAL In52Al48As_fixed.conduction.C1.<valley>.<mechanism> REMOVE
```

## Chapter 18: Indium Aluminum Arsenide Material Model

### Conduction Band Model

Table 276 Scattering mechanisms for L-minima

Scattering mechanism	L1	L2	L3	L4	L5	L6	L7	L8
	Mechanism name							
Acoustic Phonon (elastic)	ac	ac	ac	ac	ac	ac	ac	ac
Polar Optical (intra)	pop	pop	pop	pop	pop	pop	pop	pop
Optical Phonon (intra)	opl	opl	opl	opl	opl	opl	opl	opl
Optical Phonon (inter)	opl2	opl1						
Optical Phonon (inter)	opl3	opl3	opl2	opl2	opl2	opl2	opl2	opl2
Optical Phonon (inter)	opl4	opl4	opl4	opl3	opl3	opl3	opl3	opl3
Optical Phonon (inter)	opl5	opl5	opl5	opl5	opl4	opl4	opl4	opl4
Optical Phonon (inter)	opl6	opl6	opl6	opl6	opl6	opl5	opl5	opl5
Optical Phonon (inter)	opl7	opl7	opl7	opl7	opl7	opl7	opl6	opl6
Optical Phonon (inter)	opl8	opl8	opl8	opl8	opl8	opl8	opl8	opl7
Optical Phonon (inter)	opx1	opx1	opx1	opx1	opx1	opx1	opx1	opx1
Optical Phonon (inter)	opx2	opx2	opx2	opx2	opx2	opx2	opx2	opx2
Optical Phonon (inter)	opx3	opx3	opx3	opx3	opx3	opx3	opx3	opx3
Optical Phonon (inter)	opx4	opx4	opx4	opx4	opx4	opx4	opx4	opx4
Optical Phonon (inter)	opx5	opx5	opx5	opx5	opx5	opx5	opx5	opx5
Optical Phonon (inter)	opx6	opx6	opx6	opx6	opx6	opx6	opx6	opx6
Optical Phonon (inter)	opg	opg	opg	opg	opg	opg	opg	opg
Ionized Impurity	II	II	II	II	II	II	II	II
Surface Roughness	SR	SR	SR	SR	SR	SR	SR	SR
Remote Coulomb	RC	RC	RC	RC	RC	RC	RC	RC

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each  $L$ -minimum, listed in [Table 276](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL In52Al48As_fixed.conduction.C1.<valley>.<mechanism>.<parameter>
<value>
```

### Inelastic Acoustic Phonon Scattering

[Table 277](#) lists the default parameter values of the intravalley inelastic longitudinal acoustic phonon scattering.

*Table 277 Parameters of inelastic longitudinal acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	ac								
<b>Description</b>											<b>Default</b>
$\Delta_{ac}$	D	Acoustic deformation	6.376								eV
$v$	v	Velocity		3.81×10 <sup>3</sup>							m/s
$i$	final	Final minima	L1	L2	L3	L4	L5	L6	L7	L8	–

### Polar-Optical Phonon Scattering

[Table 278](#) lists the default parameter values of intravalley polar-optical phonon scattering.

*Table 278 Parameters of polar-optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	pop								
<b>Description</b>											<b>Default</b>
$E_{op}$	E	Phonon energy		39.6×10 <sup>-3</sup>							eV
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]								–

## Chapter 18: Indium Aluminum Arsenide Material Model

### Conduction Band Model

#### Optical Phonon Scattering

Table 279 to Table 282 list the default parameter values of intravalley and intervalley optical phonon scattering.

Table 279 Parameters of intravalley optical phonon scattering

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opl								
		Description	Default								
$E_{op}$	E	Phonon energy	32.7	$\times 10^{-3}$							eV
$D_{op}$	Cc	Coupling constant	1.147	$\times 10^{10}$							eV/m
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]								

Table 280 Parameters of intervalley L to L optical phonon scattering

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opl[1, 2, 3, 4, 5, 6, 7, 8]								
		Description	Default								
$E_{op}$	E	Phonon energy	22.9452	$\times 10^{-3}$							eV
$D_{op}$	Cc	Coupling constant	7.1516	$\times 10^{10}$							eV/m
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]								

## Chapter 18: Indium Aluminum Arsenide Material Model

### Conduction Band Model

Table 281 Parameters of intervalley L to X optical phonon scattering

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opx[1, 2, 3, 4, 5, 6]								
		Description	Default								
$E_{\text{op}}$	E	Phonon energy	20.2292	$\times 10^{-3}$							eV
$D_{\text{op}}$	Cc	Coupling constant	6.0892	$\times 10^{10}$							eV/m
$i$	final	Final minima	X	[1, 2, 3, 4, 5, 6]							—

Table 282 Parameters of intervalley L to  $\Gamma$  optical phonon scattering

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opg								
		Description	Default								
$E_{\text{op}}$	E	Phonon energy	21.1076	$\times 10^{-3}$							eV
$D_{\text{op}}$	Cc	Coupling constant	6.2764	$\times 10^{10}$							eV/m
$i$	final	Final minima	G								—

## $\Gamma$ -Valley Scattering Mechanisms

The  $\Gamma$ -minimum defines the set of scattering mechanisms listed in Table 283. By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL In52Al48As_fixed.conduction.C2.G.<mechanism> ADD
```

```
MATERIAL In52Al48As_fixed.conduction.C2.G.<mechanism> REMOVE
```

**Chapter 18: Indium Aluminum Arsenide Material Model**  
Conduction Band Model

*Table 283 Scattering mechanisms for  $\Gamma$ -minimum*

Scattering mechanism	Mechanism name
Acoustic Phonon (elastic)	ac
Polar Optical (intra)	pop
Optical Phonon (inter)	opl1
Optical Phonon (inter)	opl2
Optical Phonon (inter)	opl3
Optical Phonon (inter)	opl4
Optical Phonon (inter)	opl5
Optical Phonon (inter)	opl6
Optical Phonon (inter)	opl7
Optical Phonon (inter)	opl8
Optical Phonon (inter)	opx1
Optical Phonon (inter)	opx2
Optical Phonon (inter)	opx3
Optical Phonon (inter)	opx4
Optical Phonon (inter)	opx5
Optical Phonon (inter)	opx6
Ionized Impurity	II
Surface Roughness	SR
Remote Coulomb	RC

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for the  $\Gamma$ -minimum, listed in [Table 283](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL In52Al48As_fixed.conduction.C2.G.<mechanism>. <parameter> <value>
```

### Inelastic Acoustic Phonon Scattering

[Table 284](#) lists the default parameter values of intravalley inelastic *longitudinal* acoustic phonon scattering.

*Table 284 Parameters of inelastic longitudinal acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	ac	
		Description	Default	
$\Delta_{ac}$	D	Acoustic deformation	6.376	eV
$v$	v	Velocity	$3.81 \times 10^3$	m/s
$i$	final	Final minima	G	—

### Polar-Optical Phonon Scattering

[Table 285](#) lists the default parameter values of intravalley polar-optical phonon scattering.

*Table 285 Parameters of polar-optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	pop	
		Description	Default	
$E_{op}$	E	Phonon energy	$39.6 \times 10^{-3}$	eV
$i$	final	Final minima	G	—

## Chapter 18: Indium Aluminum Arsenide Material Model

### Conduction Band Model

#### Optical Phonon Scattering

[Table 286](#) and [Table 287](#) list the default parameter values of intervalley optical phonon scattering.

*Table 286 Parameters of intervalley  $\Gamma$  to L optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
<b>Mechanism name:</b> opl[1, 2, 3, 4, 5, 6, 7, 8]				
<b>Description</b>				<b>Default</b>
$E_{\text{op}}$	E	Phonon energy	$21.107 \times 10^{-3}$	eV
$D_{\text{op}}$	Cc	Coupling constant	$6.2764 \times 10^{10}$	eV/m
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]	—

*Table 287 Parameters for intervalley  $\Gamma$  to X optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
<b>Mechanism name:</b> opx[1, 2, 3, 4, 5, 6]				
<b>Description</b>				<b>Default</b>
$E_{\text{op}}$	E	Phonon energy	$22.0332 \times 10^{-3}$	eV
$D_{\text{op}}$	Cc	Coupling constant	$6.806 \times 10^{10}$	eV/m
$i$	final	Final minima	X[1, 2, 3, 4, 5, 6]	—

---

## Ionized Impurity Scattering

Ionized impurity scattering is defined for each valley in a conduction band and is treated as an intravalley process by default, so that the final valley after scattering is the same as the initial valley.

*Table 288 Parameters of ionized impurity scattering*

Parameter symbol	Parameter name	Valley name:	All valleys	Unit
		<b>Mechanism name:</b>	II	
		<b>Description</b>	<b>Default</b>	
<i>i</i>	final	Final minimum	Same as initial minimum	–

## Ionized Impurity Empirical Rate Factor

The ionized impurity scattering model includes a scaling factor for the empirical correction of the calculated scattering rate as a function of doping density.

To redefine the default empirical factor, use the following input file syntax:

```
MATERIAL In52Al48As_fixed.conduction.IIfac N <Nvalue> [<Nvalue2>] <rule>
<value>
```

Here, **IIfac** is a piecewise interpolation parameter that defines a correction factor **<value>** for a value **<Nvalue>** of the doping concentration **N**. The interpolation model used to return values between specified densities is given by **<rule>**, which might require an upper bound of the density [**<Nvalue2>**]. For a description of the interpolation parameter type, see [Interpolation Methods on page 301](#).

By default, the empirical correction for ionized impurity is 1.0. However, for electrons in  $\text{In}_{52}\text{Al}_{48}\text{As}$ , a non-unity default value is provided to best match experimental low-field concentration-dependent mobility.

---

## Surface Roughness Scattering

**Table 289** lists the default parameter values of surface roughness scattering. These parameters apply to all valleys and to all equivalent surface orientations.

*Table 289 Parameters of surface roughness scattering*

Parameter symbol	Parameter name	Mechanism name:	SR		Unit
		Description	Default		
$\Delta$	rms	RMS amplitude	1.2	1.2	nm
$L_c$	l	Correlation length	1.0	1.0	nm
$\langle hkl \rangle$	orient	Surface orientation	(001)	(110)	–
$i$	carrier	Carrier type	electrons	electrons	–

---

## Remote Coulomb Scattering

**Table 290** lists the default parameter values of remote Coulomb scattering, which is treated as an intravalley process. These parameters apply to all valleys.

*Table 290 Parameters of remote Coulomb scattering*

Parameter symbol	Parameter name	Mechanism name:	RC		Unit
		Description	Default		
$z_d$	zd	Depth of charge centroid	1.5		nm
$E_0$	e0	Minimum energy for tabulating rate	0		eV
$N_0$	n0	Minimum screening density	$5 \times 10^{15}$		$\text{cm}^{-3}$
$i$	final	Final minimum	Same as initial minimum		–

To define the interface charge density for remote Coulomb scattering, follow the descriptions in [Defining Interface Models on page 217](#). By default, no interface charge is applied.

## Chapter 18: Indium Aluminum Arsenide Material Model

### Valence Band Model

---

## Valence Band Model

This section describes the valence band model.

---

### Band Edge Parameters

To change the default parameter values of the valence band container model, listed in [Table 291](#), use the following input file syntax:

```
MATERIAL In52Al48As_fixed.valence.<parameter> <value>
```

*Table 291 Parameters of valence band container model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Valence band energy with respect to vacuum	5.7576	eV
$m_{dg_x}$	$dgx$	Hole density gradient effective x-mass	0.5	$m_e$
$m_{dg_y}$	$dgy$	Hole density gradient effective y-mass	0.5	$m_e$
$m_{dg_z}$	$dgz$	Hole density gradient effective z-mass	0.5	$m_e$
k·p band structure model parameters				
$L$	$L-kp$	Valence band parameter	0.0	$\hbar^2/2m$
$M$	$M-kp$	Valence band parameter	0.0	$\hbar^2/2m$
$N$	$N-kp$	Valence band parameter	0.0	$\hbar^2/2m$
$l$	$l-defpot$	Valence deformation potential	0.0	eV
$m$	$m-defpot$	Valence deformation potential	0.0	eV
$n$	$n-defpot$	Valence deformation potential	0.0	eV
$\Delta_{sso}$	$dsso$	Spin-orbit split energy	0.0	eV

## Chapter 18: Indium Aluminum Arsenide Material Model

### Valence Band Model

To change the default parameter values of the valence bands in the container model, listed in [Table 292](#), use the following input file syntax:

```
MATERIAL Silicon.valence.<band>.<parameter> <value>
```

*Table 292 Parameters of valence band model*

Parameter symbol	Parameter name	Description	Default	Unit
Heavy hole (HH) band				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.0	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	6kp	—
Light hole (LH) band				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.0	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	6kp	—
Spin split-off (SSO) band				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.044	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	6kp	—

## Mobility Models

The valence band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models together with some phenomenological enhancement factors.

### Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 293](#), use the following input file syntax:

```
MATERIAL In52Al48As_fixed.valence.constant.<parameter> <value>
```

## Chapter 18: Indium Aluminum Arsenide Material Model

### Valence Band Model

Table 293 Parameters of constant mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	200	$\text{cm}^2/\text{Vs}$
$\zeta$	zeta	Fitting parameter	2.2	—

## Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 294](#), use the following input file syntax:

```
MATERIAL In52Al48As_fixed.valence.Arora.<parameter> <value>
```

Table 294 Parameters of Arora mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min}$	mumin	Minimum mobility	54.3	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	200	$\text{cm}^2/\text{Vs}$
$N_0$	n0	Reference concentration	$2.35 \times 10^{17}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.88	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.33	—
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

## Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 295](#), use the following input file syntax:

```
MATERIAL In52Al48As_fixed.valence.Masetti.<parameter> <value>
```

## Chapter 18: Indium Aluminum Arsenide Material Model

### Valence Band Model

Table 295 Parameters of Masetti mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min 1}$	mumin1	Minimum mobility	40.0	$\text{cm}^2/\text{Vs}$
$\mu_{\min 2}$	mumin2	Minimum mobility	40.0	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	200	$\text{cm}^2/\text{Vs}$
$\mu_1$	mul	Maximum mobility	1.0	$\text{cm}^2/\text{Vs}$
$C_r$	cr	Reference concentration	$2.23 \times 10^{17}$	$\text{cm}^{-3}$
$C_s$	cs	Reference solid solubility concentration	$3.80 \times 10^{17}$	$\text{cm}^{-3}$
$p_c$	pc	Reference concentration	0.0	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.719	—
$\beta$	beta	Fitting parameter	2.0	—
$\zeta$	zeta	Fitting parameter	2.2	—

## Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 296](#), use the following input file syntax:

```
MATERIAL In52Al48As_fixed.valence.Yamaguchi.<parameter> <value>
```

Table 296 Parameters of Yamaguchi mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

## Chapter 18: Indium Aluminum Arsenide Material Model

### Valence Band Model

## Perpendicular Field: Lombardi Mobility Model

To change the default parameter values of the Lombardi mobility model, listed in [Table 297](#), use the following input file syntax:

```
MATERIAL In52Al48As_fixed.valence.Lombardi.<parameter> <value>
```

*Table 297 Parameters of Lombardi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
A	a	Fitting parameter	2.0	—
B	b	Fitting parameter	$9.925 \times 10^6$	cm/s
C	c	Fitting parameter	$2.947 \times 10^3$	$\text{cm}^{5/3} \text{V}^{-2/3} \text{s}^{-1}$
$\alpha$	alpha	Fitting parameter	0.0	$\text{cm}^3$
$\delta$	delta	Fitting parameter	$2.0546 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$2.0546 \times 10^{30}$	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	1.0	—
$\lambda$	lambda	Fitting parameter	0.0317	—
$\nu$	nu	Fitting parameter	1.0	—
$N_0$	n0	Fitting parameter	1.0	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	1.0	$\text{cm}^{-3}$
$l_{\text{crit}}$	lcrit	Critical length	$1 \times 10^{-6}$	cm

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in [Table 298](#), use the following input file syntax:

```
MATERIAL In52Al48As_fixed.valence.Caughey.<parameter> <value>
```

## Chapter 18: Indium Aluminum Arsenide Material Model

### Valence Band Model

Table 298 Parameters of Caughey–Thomas mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$8.37 \times 10^6$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	0.52	—
$\beta_0$	beta0	Fitting parameter	1.213	—
$\beta_{\text{exp}}$	bexp	Fitting parameter	0.17	—
$\alpha$	alpha	Fitting parameter	0.0	—

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 299](#). To change the default mobility model, use the following input file syntax:

```
MATERIAL In52Al48As_fixed.valence.mobility.<model> <value>
```

Table 299 Parameters of default mobility model

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley valence band model consists of the valley minima listed in [Table 300](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL In52Al48As_fixed.valence.<band>.<valley> REMOVE
```

### Note:

The valence band analytic valley approximation is used only as a way to define density-of-states for drift-diffusion simulations and to define the valley minima in response to stress.

## Chapter 18: Indium Aluminum Arsenide Material Model

### Valence Band Model

*Table 300 Names of valence band minima*

Valence band minima	Band name	Valley name
Heavy hole	HH	vhh
Light hole	LH	vlh
Spin split-off	SSO	vsso

## Position and Orientation

The position and orientation of the HH, LH, and SSO valley minima are identical. [Table 301](#) shows the default values. To change the default values, use the following input file syntax:

```
MATERIAL In52Al48As_fixed.valence.<band>.<valley>.min.<parameter> <value>
```

*Table 301 Position and orientation parameters of HH, LH, and SSO valley minima*

Parameter symbol	Parameter name	Description	Default	Unit
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.0	$2\pi/a$
x	x	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
y	y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
z	z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$

## Parameters

To change the valley minima model parameters, listed in [Table 302](#), for each valley listed in [Table 300](#), use the following input file syntax:

```
MATERIAL In52Al48As_fixed.valence.<band>.<valley>.<parameter> <value>
```

*Table 302 Parameters of valence band minima*

Parameter symbol	Parameter name	Description	Default	Unit
<b>Heavy hole (HH) band</b>				
E	E	Minima with respect to band edge	0.0	eV

## Chapter 18: Indium Aluminum Arsenide Material Model

### Valence Band Model

Table 302 Parameters of valence band minima (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$m_x$	mx	Longitudinal effective mass	0.578	$m_e$
$m_y$	my	Transverse effective mass	0.578	$m_e$
$m_z$	mz	Transverse effective mass	0.578	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	0.0	eV
<b>Light hole (LH) band</b>				
$E$	E	Minima with respect to band edge	0.0	eV
$m_x$	mx	Longitudinal effective mass	0.0855	$m_e$
$m_y$	my	Transverse effective mass	0.0855	$m_e$
$m_z$	mz	Transverse effective mass	0.0855	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	0.0	eV
<b>Spin split-off (SSO) band</b>				
$E$	E	Minima with respect to band edge	0.2998	eV
$m_x$	mx	Longitudinal effective mass	0.3416	$m_e$
$m_y$	my	Transverse effective mass	0.3416	$m_e$
$m_z$	mz	Transverse effective mass	0.3416	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	0.0	eV

## **Heavy-Hole Band Scattering Mechanisms**

There are no heavy-hole band scattering mechanisms defined in the current version of Garand.

---

## **Light-Hole Band Scattering Mechanisms**

There are no light-hole band scattering mechanisms defined in the current version of Garand.

---

## **Spin Split-Off Band Scattering Mechanisms**

There are no spin split-off band scattering mechanisms defined in the current version of Garand.

---

## **Simulation Results**

This section presents various simulation results for the  $\text{In}_{52}\text{Al}_{48}\text{As}$  material model.

---

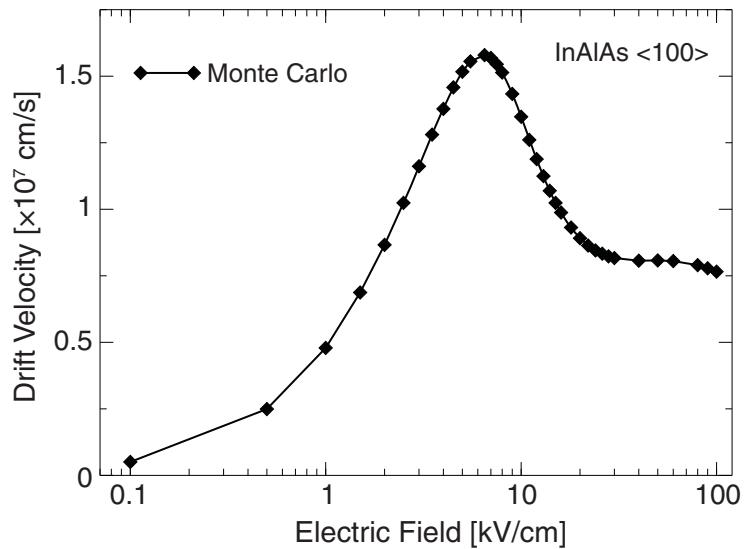
## **Velocity-Field Characteristics**

[Figure 51](#) shows the velocity-field characteristics of InAlAs material, calibrated to experimental data for InGaAs (with fractions of  $\text{In}_{0.52}\text{Al}_{0.48}\text{As}$ ), at 300 K from Monte Carlo simulation.

## Chapter 18: Indium Aluminum Arsenide Material Model

### Simulation Results

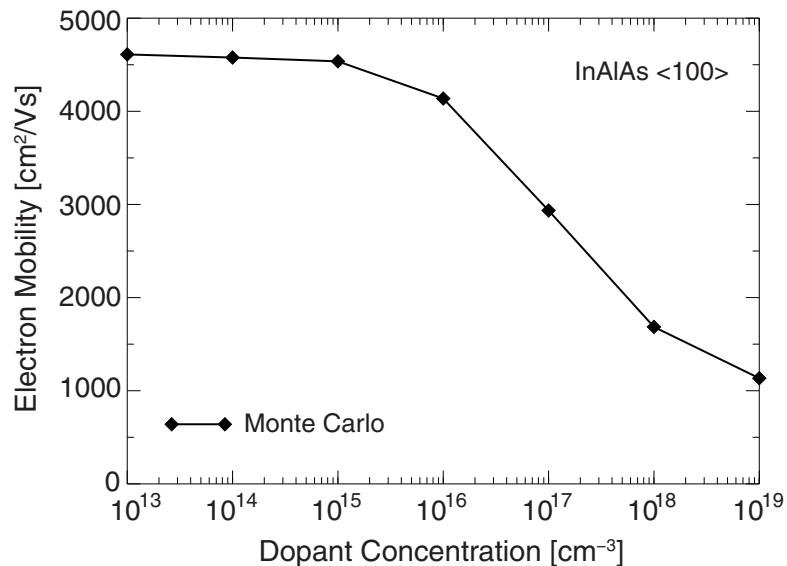
Figure 51 Simulated velocity-field characteristics for InAlAs material



### Low-Field Concentration-Dependent Mobility

Figure 52 shows the simulated low-field electron mobility in InAlAs (with fractions of  $\text{In}_{0.52}\text{Al}_{0.48}\text{As}$ ) at 300 K.

Figure 52 Simulated doping-dependent low-field electron mobility in InAlAs



## Gallium Arsenide Material Model

---

*This chapter describes the GaAs material model.*

---

### Bulk Material Model

This section describes the bulk material model for GaAs.

---

#### Parameters of Bulk Material Model

To change the default parameter values in [Table 303](#), use the following input file syntax:

```
MATERIAL GaAs.<parameter> <value>
```

*Table 303 Bulk material model parameters*

Parameter symbol	Parameter name	Description	Default	Unit
<b>Crystal lattice and orientation in simulation domain</b>				
a	a	Magnitude of lattice vector a	5.65325	Å
b	b	Magnitude of lattice vector b	5.65325	Å
c	c	Magnitude of lattice vector c	5.65325	Å
$\alpha$	alpha	Angle between b and c	90	degree
$\beta$	beta	Angle between c and a	90	degree
$\gamma$	gamma	Angle between a and b	90	degree
$\langle hkl \rangle_x$	x	Orientation in the x-direction	1 0 0	–

## Chapter 19: Gallium Arsenide Material Model

### Bulk Material Model

*Table 303 Bulk material model parameters (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$\langle hkl \rangle_z$	z	Orientation in the z-direction	0 0 1	–
<b>Bulk electrical and mechanical properties</b>				
$\kappa$	permittivity	Relative dielectric constant	12.90	–
$\kappa_\infty$	k_inf	High-frequency permittivity	10.89	–
$\rho$	density	Mass density	5.32	g/cm <sup>3</sup>
$C_{11}$	c11	Elastic stiffness matrix element	119.0	GPa
$C_{12}$	c12	Elastic stiffness matrix element	53.4	GPa
$C_{44}$	c44	Elastic stiffness matrix element	59.6	GPa

## Band-to-Band Tunneling Parameters

To change the default parameter values for the Kane model, listed in [Table 304](#), use the following input file syntax:

```
MATERIAL GaAs.BTBT.<parameter> <value>
```

*Table 304 Band-to-band tunneling parameters*

Parameter symbol	Parameter name	Description	Default	Unit
$D_{TA}$	DTA	Acoustic phonon deformation potential	0.0	eV
$\epsilon_{TA}$	epsilonTA	Acoustic phonon energy	0.0	eV

## Chapter 19: Gallium Arsenide Material Model

### Conduction Band Model

---

## Conduction Band Model

This section describes the conduction band model.

---

### Band Edge Parameters

To change the default parameter values of the conduction band container model, listed in [Table 305](#), use the following input file syntax:

```
MATERIAL GaAs.conduction.<parameter> <value>
```

*Table 305 Parameters of conduction band container model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Conduction band energy with respect to vacuum	4.07	eV
$m_{dg_x}$	$dgx$	Electron density gradient effective x-mass	0.3	$m_e$
$m_{dg_y}$	$dgy$	Electron density gradient effective y-mass	0.3	$m_e$
$m_{dg_z}$	$dgz$	Electron density gradient effective z-mass	0.3	$m_e$

To change the default parameter values of the conduction bands in the container model, listed in [Table 306](#), use the following input file syntax:

```
MATERIAL GaAs.conduction.<band>.<parameter> <value>
```

*Table 306 Parameters of conduction band model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Conduction band energy with respect to container energy	0.0	eV
$model$	$model$	Model used for transport in this band	ema	—

---

## Mobility Models

The conduction band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models.

### Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 307](#), use the following input file syntax:

```
MATERIAL GaAs.conduction.constant.<parameter> <value>
```

*Table 307 Parameters of constant mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	$9.4 \times 10^3$	$\text{cm}^2/\text{Vs}$
$\zeta$	zeta	Fitting parameter	2.1	—

### Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 308](#), use the following input file syntax:

```
MATERIAL GaAs.conduction.Arora.<parameter> <value>
```

*Table 308 Parameters of Arora mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min}$	mumin	Minimum mobility	88.0	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	$9.4 \times 10^3$	$\text{cm}^2/\text{Vs}$
$N_0$	n0	Reference concentration	$1.25 \times 10^{17}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.88	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.33	—

## Chapter 19: Gallium Arsenide Material Model

### Conduction Band Model

*Table 308 Parameters of Arora mobility model (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

## Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 309](#), use the following input file syntax:

```
MATERIAL GaAs.conduction.Masetti.<parameter> <value>
```

*Table 309 Parameters of Masetti mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min 1}$	mumin1	Minimum mobility	220.0	$\text{cm}^2/\text{Vs}$
$\mu_{\min 2}$	mumin2	Minimum mobility	220.0	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	$9.4 \times 10^3$	$\text{cm}^2/\text{Vs}$
$\mu_1$	mul	Maximum mobility	1.0	$\text{cm}^2/\text{Vs}$
$C_r$	cr	Reference concentration	$1.2 \times 10^{17}$	$\text{cm}^{-3}$
$C_s$	cs	Reference solid solubility concentration	0.0	$\text{cm}^{-3}$
$p_c$	pc	Reference concentration	0.0	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.5	—
$\beta$	beta	Fitting parameter	2.0	—
$\zeta$	zeta	Fitting parameter	2.1	—

## Chapter 19: Gallium Arsenide Material Model

### Conduction Band Model

## Low Field: Philips Unified Mobility Model

To change the default parameter values of the Philips unified mobility model, listed in [Table 310](#), use the following input file syntax:

```
MATERIAL GaAs.conduction.Philips.<parameter> <value>
```

*Table 310 Parameters of Philips unified mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min}$	mumin	Minimum mobility	55.2	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	$9.4 \times 10^3$	$\text{cm}^2/\text{Vs}$
$\alpha$	alpha	Fitting parameter	0.68	—
$C_D$	CD	Reference concentration for ultrahigh-doped donors	0.21	—
$C_A$	CA	Reference concentration for ultrahigh-doped acceptors	0.5	—
$N_{\text{ref}}$	Nref	Reference concentration	$9.68 \times 10^{16}$	$\text{cm}^{-3}$
$N_{D, \text{ref}}$	NDref	Reference concentration	$4.0 \times 10^{20}$	$\text{cm}^{-3}$
$N_{A, \text{ref}}$	NAref	Reference concentration	$7.2 \times 10^{20}$	$\text{cm}^{-3}$
$N_{c, \text{ref}}$	Ncref	Reference concentration	$1.36 \times 10^{20}$	$\text{cm}^{-3}$
$N_{sc, \text{ref}}$	Nscref	Reference surface concentration	$3.97 \times 10^{13}$	$\text{cm}^{-2}$
$m_e$	me	Normalized electron mass	1.0	—
$m_h$	mh	Normalized hole mass	1.25	—
$f_{BH}$	fbh	Brooks–Herring coefficient	3.828	—
$f_{CW}$	fcw	Conwell–Weisskopf coefficient	2.459	—

## Chapter 19: Gallium Arsenide Material Model

### Conduction Band Model

## Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 311](#), use the following input file syntax:

```
MATERIAL GaAs.conduction.Yamaguchi.<parameter> <value>
```

*Table 311 Parameters of Yamaguchi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

## Perpendicular Field: Lombardi Mobility Model

To change the default parameter values of the Lombardi mobility model, listed in [Table 312](#), use the following input file syntax:

```
MATERIAL GaAs.conduction.Lombardi.<parameter> <value>
```

*Table 312 Parameters of Lombardi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$A$	a	Fitting parameter	2.0	—
$B$	b	Fitting parameter	$4.75 \times 10^7$	cm/s
$C$	c	Fitting parameter	$5.80 \times 10^2$	$\text{cm}^{5/3} \text{V}^{-2/3} \text{s}^{-1}$
$\alpha$	alpha	Fitting parameter	0.0	$\text{cm}^3$
$\delta$	delta	Fitting parameter	$5.82 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$5.82 \times 10^{30}$	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	1.0	—
$\lambda$	lambda	Fitting parameter	0.125	—
$\nu$	nu	Fitting parameter	1.0	—

## Chapter 19: Gallium Arsenide Material Model

### Conduction Band Model

Table 312 Parameters of Lombardi mobility model (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$N_0$	n0	Fitting parameter	1.0	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	1.0	$\text{cm}^{-3}$
$l_{\text{crit}}$	lcrit	Critical length	$1 \times 10^{-6}$	cm

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in [Table 313](#), use the following input file syntax:

```
MATERIAL GaAs.conduction.Caughey.<parameter> <value>
```

Table 313 Parameters of Caughey–Thomas mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$6.0 \times 10^6$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	0.87	—
$\beta_0$	beta0	Fitting parameter	1.109	—
$\beta_{\text{exp}}$	bexp	Fitting parameter	0.66	—
$\alpha$	alpha	Fitting parameter	0.0	—

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 314](#). To change the default mobility model, use the following input file syntax:

```
MATERIAL GaAs.conduction.mobility.<model> <value>
```

## Chapter 19: Gallium Arsenide Material Model

### Conduction Band Model

Table 314 Parameters of default mobility model

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley conduction band model consists of the valley minima listed in [Table 315](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL GaAs.conduction.<band>.<valley> REMOVE
```

Table 315 Names of conduction band C1 minima

Conduction band minimum	Valley name
X	X1, X2, X3, X4, X5, X6
L	L1, L2, L3, L4, L5, L6, L7, L8
$\Gamma$	G

## Position and Orientation

Valley minima differ in their position and orientation, the default values of which are shown in [Table 316](#), [Table 317](#), and [Table 318](#).

To change default values, use the following input file syntax:

```
MATERIAL GaAs.conduction.C1.<valley>.min.<parameter> <value>
```

Table 316 Position and orientation parameters of X-minima of conduction band

Parameter symbol	Parameter name	Description	Default	Unit
<b>X1</b>				
$k_0$	pos	Position within the Brillouin zone	1.0 0.0 0.0	$2\pi/a$

## Chapter 19: Gallium Arsenide Material Model

### Conduction Band Model

*Table 316 Position and orientation parameters of X-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$x$	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X2</b>				
$k_0$	pos	Position within the Brillouin zone	-1.0 0.0 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X3</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 1.0 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	0 1 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X4</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 -1.0 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	0 1 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X5</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 1.0	$2\pi/a$

## Chapter 19: Gallium Arsenide Material Model

### Conduction Band Model

*Table 316 Position and orientation parameters of X-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
x	X	Orientation of the x-axis	0 0 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	0 -1 0	$\langle hkl \rangle$
<b>X6</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 -1.0	$2\pi/a$
x	X	Orientation of the x-axis	0 0 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	0 -1 0	$\langle hkl \rangle$

*Table 317 Position and orientation parameters of L-minima of conduction band*

Parameter symbol	Parameter name	Description	Default	Unit
<b>L1</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 1 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L2</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 1 1	$\langle hkl \rangle$

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### Conduction Band Model

*Table 317 Position and orientation parameters of L-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
y	Y	Orientation of the y-axis	1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 1 0	$\langle hkl \rangle$
<b>L3</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 -0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 -1 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$
<b>L4</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	1 1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L5</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 -0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 -1 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 -1 -2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L6</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 1 -1	$\langle hkl \rangle$

## Chapter 19: Gallium Arsenide Material Model

### Conduction Band Model

*Table 317 Position and orientation parameters of L-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
y	Y	Orientation of the y-axis	1 -1 -2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$
<b>L7</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 -0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 -1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$
<b>L8</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 -0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 -1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 1 0	$\langle hkl \rangle$

*Table 318 Position and orientation parameters of  $\Gamma$ -minimum of conduction band*

Parameter symbol	Parameter name	Description	Default	Unit
<b>G</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.0	$2\pi/a$
x	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$

## Chapter 19: Gallium Arsenide Material Model

### Conduction Band Model

## Parameters

To change the default parameter values of the valley minima models, listed in the following tables, for each valley listed in [Table 315](#), use the following input file syntax:

```
MATERIAL GaAs.conduction.C1.<valley>.<parameter> <value>
```

### Note:

By default, all  $X$ -minima have the same parameter values, and all  $L$ -minima have the same parameter values.

*Table 319 Parameters of X-valley model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	<code>E</code>	Minima with respect to band edge	0.48	eV
$m_x$	<code>mx</code>	Longitudinal effective mass	1.3	$m_e$
$m_y$	<code>my</code>	Transverse effective mass	0.23	$m_e$
$m_z$	<code>mz</code>	Transverse effective mass	0.23	$m_e$
$\alpha$	<code>a</code>	Valley nonparabolicity factor	0.36	—
$\Xi_u$	<code>xi_u</code>	Uniaxial deformation potential	0.0	eV
$\Xi_d$	<code>xi_d</code>	Dilatation deformation potential	0.0	eV
$\Xi'_u$	<code>xi_u_prime</code>	Uniaxial mass deformation	0.0	eV

*Table 320 Parameters of L-valley model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	<code>E</code>	Minima with respect to band edge	0.29	eV
$m_x$	<code>mx</code>	Longitudinal effective mass	1.9	$m_e$
$m_y$	<code>my</code>	Transverse effective mass	0.0754	$m_e$

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### Conduction Band Model

Table 320 Parameters of L-valley model (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$m_z$	mxz	Transverse effective mass	0.0754	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.4	—
$\Xi_u$	xi_u	Uniaxial deformation potential	0.0	eV
$\Xi_d$	xi_d	Dilatation deformation potential	0.0	eV
$\Xi'_u$	xi_u_prime	Uniaxial mass deformation	0.0	eV

Table 321 Parameters of  $\Gamma$ -valley model

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Minima with respect to band edge	0.0	eV
$m_x$	mx	Longitudinal effective mass	0.063	$m_e$
$m_y$	my	Transverse effective mass	0.063	$m_e$
$m_z$	mxz	Transverse effective mass	0.063	$m_e$
$\alpha$	a	Valley nonparabolicity factor	1.16	—
$\Xi_u$	xi_u	Uniaxial deformation potential	0.0	eV
$\Xi_d$	xi_d	Dilatation deformation potential	0.0	eV
$\Xi'_u$	xi_u_prime	Uniaxial mass deformation	0.0	eV

## X-Valley Scattering Mechanisms

The six X-minima define the set of scattering mechanisms listed in Table 322. By default, all these scattering mechanisms are added to the default scattering model. To change the

## Chapter 19: Gallium Arsenide Material Model

### Conduction Band Model

default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL GaAs.conduction.C1.<valley>.<mechanism> ADD
```

```
MATERIAL GaAs.conduction.C1.<valley>.<mechanism> REMOVE
```

Table 322 Scattering mechanisms for X-minima

Scattering mechanism	X1	X2	X3	X4	X5	X6
	Mechanism name					
Acoustic Phonon (elastic)	ac	ac	ac	ac	ac	ac
Polar Optical (intra)	pop	pop	pop	pop	pop	pop
Optical Phonon (inter)	opx2	opx1	opx1	opx1	opx1	opx1
Optical Phonon (inter)	opx3	opx3	opx2	opx3	opx3	opx3
Optical Phonon (inter)	opx4	opx4	opx4	opx2	opx4	opx4
Optical Phonon (inter)	opx5	opx5	opx5	opx5	opx2	opx5
Optical Phonon (inter)	opx6	opx6	opx6	opx6	opx6	opx2
Optical Phonon (inter)	opl1	opl1	opl1	opl1	opl1	opl1
Optical Phonon (inter)	opl2	opl2	opl2	opl2	opl2	opl2
Optical Phonon (inter)	opl3	opl3	opl3	opl3	opl3	opl3
Optical Phonon (inter)	opl4	opl4	opl4	opl4	opl4	opl4
Optical Phonon (inter)	opl5	opl5	opl5	opl5	opl5	opl5
Optical Phonon (inter)	opl6	opl6	opl6	opl6	opl6	opl6
Optical Phonon (inter)	opl7	opl7	opl7	opl7	opl7	opl7
Optical Phonon (inter)	opl8	opl8	opl8	opl8	opl8	opl8
Optical Phonon (inter)	opg	opg	opg	opg	opg	opg
Ionized Impurity	II	II	II	II	II	II

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### Conduction Band Model

Table 322 Scattering mechanisms for X-minima (Continued)

Scattering mechanism	X1	X2	X3	X4	X5	X6
<b>Mechanism name</b>						
Surface Roughness	SR	SR	SR	SR	SR	SR
Remote Coulomb	RC	RC	RC	RC	RC	RC

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each  $X$ -minimum, listed in [Table 322](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL GaAs.conduction.C1.<valley>.<mechanism>.<parameter> <value>
```

## Elastic Acoustic Phonon Scattering

[Table 323](#) lists the default parameter values of intravalley elastic acoustic phonon scattering.

Table 323 Parameters of elastic acoustic phonon scattering

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
<b>Mechanism name: ac</b>									
<b>Description</b>									<b>Default</b>
$\Delta_{ac}$	D	Acoustic deformation	5.0						eV
$v$	v	Velocity		3.86×10 <sup>3</sup>					m/s
$i$	final	Final minima	X1	X2	X3	X4	X5	X6	–

## Chapter 19: Gallium Arsenide Material Model

Conduction Band Model

### Polar-Optical Phonon Scattering

[Table 324](#) lists the default parameter values of intravalley polar-optical phonon scattering.

*Table 324 Parameters of polar-optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit		
		Mechanism name:	pop								
		Description	Default								
$E_{op}$	E	Phonon energy			$37.798 \times 10^{-3}$				eV		
$i$	final	Final minima	X1	X2	X3	X4	X5	X6	—		

### Optical Phonon Scattering

[Table 325](#) to [Table 327](#) list the default parameter values of intervalley optical phonon scattering.

*Table 325 Parameters of intervalley X to X optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit		
		Mechanism name:	opx [1, 2, 3, 4, 5, 6]								
		Description	Default								
$E_{op}$	E	Phonon energy			$24.31 \times 10^{-3}$				eV		
$D_{op}$	Cc	Coupling constant			$2.99 \times 10^{10}$				eV/m		
$i$	final	Final minima			$X[1, 2, 3, 4, 5, 6]$				—		

## Chapter 19: Gallium Arsenide Material Model

### Conduction Band Model

Table 326 Parameters of intervalley X to L optical phonon scattering

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
<b>Mechanism name: opl[1, 2, 3, 4, 5, 6, 7, 8]</b>									
<b>Description</b>									<b>Default</b>
$E_{op}$	E	Phonon energy	$21.85 \times 10^{-3}$						
$D_{op}$	Cc	Coupling constant	$3.284 \times 10^{11}$						
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]						

Table 327 Parameters of intervalley X to  $\Gamma$  optical phonon scattering

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
<b>Mechanism name: opg</b>									
<b>Description</b>									<b>Default</b>
$E_{op}$	E	Phonon energy	$23.45 \times 10^{-3}$						
$D_{op}$	Cc	Coupling constant	$2.454 \times 10^{11}$						
$i$	final	Final minima	G						

## L-Valley Scattering Mechanisms

The eight L-minima define the set of scattering mechanisms listed in Table 328. By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL GaAs.conduction.C1.<valley>.<mechanism> ADD
```

```
MATERIAL GaAs.conduction.C1.<valley>.<mechanism> REMOVE
```

## Chapter 19: Gallium Arsenide Material Model

### Conduction Band Model

Table 328 Scattering mechanisms for L-minima

Scattering mechanism	L1	L2	L3	L4	L5	L6	L7	L8
	Mechanism name							
Acoustic Phonon (elastic)	ac	ac	ac	ac	ac	ac	ac	ac
Polar Optical (intra)	pop	pop	pop	pop	pop	pop	pop	pop
Optical Phonon (intra)	opl	opl	opl	opl	opl	opl	opl	opl
Optical Phonon (inter)	opl2	opl1						
Optical Phonon (inter)	opl3	opl3	opl2	opl2	opl2	opl2	opl2	opl2
Optical Phonon (inter)	opl4	opl4	opl4	opl3	opl3	opl3	opl3	opl3
Optical Phonon (inter)	opl5	opl5	opl5	opl5	opl4	opl4	opl4	opl4
Optical Phonon (inter)	opl6	opl6	opl6	opl6	opl6	opl5	opl5	opl5
Optical Phonon (inter)	opl7	opl7	opl7	opl7	opl7	opl7	opl6	opl6
Optical Phonon (inter)	opl8	opl8	opl8	opl8	opl8	opl8	opl8	opl7
Optical Phonon (inter)	opx1	opx1	opx1	opx1	opx1	opx1	opx1	opx1
Optical Phonon (inter)	opx2	opx2	opx2	opx2	opx2	opx2	opx2	opx2
Optical Phonon (inter)	opx3	opx3	opx3	opx3	opx3	opx3	opx3	opx3
Optical Phonon (inter)	opx4	opx4	opx4	opx4	opx4	opx4	opx4	opx4
Optical Phonon (inter)	opx5	opx5	opx5	opx5	opx5	opx5	opx5	opx5
Optical Phonon (inter)	opx6	opx6	opx6	opx6	opx6	opx6	opx6	opx6
Optical Phonon (inter)	opg	opg	opg	opg	opg	opg	opg	opg
Ionized Impurity	II	II	II	II	II	II	II	II
Surface Roughness	SR	SR	SR	SR	SR	SR	SR	SR
Remote Coulomb	RC	RC	RC	RC	RC	RC	RC	RC

## Chapter 19: Gallium Arsenide Material Model

### Conduction Band Model

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each  $L$ -minimum, listed in [Table 328](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL GaAs.conduction.C1.<valley>.<mechanism>.<parameter> <value>
```

### Elastic Acoustic Phonon Scattering

[Table 329](#) lists the default parameter values of intravalley elastic *longitudinal* acoustic phonon scattering.

*Table 329 Parameters of elastic longitudinal acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	ac								
		Description	Default								
$\Delta_{ac}$	D	Acoustic deformation	5.0								eV
$v$	v	Velocity									m/s
$i$	final	Final minima	L1	L2	L3	L4	L5	L6	L7	L8	—

### Polar-Optical Phonon Scattering

[Table 330](#) lists the default parameter values of intravalley polar-optical phonon scattering.

*Table 330 Parameters of polar-optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	pop								
		Description	Default								
$E_{op}$	E	Phonon energy									eV
$i$	final	Final minima	L1	L2	L3	L4	L5	L6	L7	L8	—

## Chapter 19: Gallium Arsenide Material Model

### Conduction Band Model

#### Optical Phonon Scattering

Table 331 to Table 334 list the default parameter values of intravalley and intervalley optical phonon scattering.

Table 331 Parameters of intravalley optical phonon scattering

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opl								
		Description	Default								
$E_{op}$	E	Phonon energy									eV
$D_{op}$	Cc	Coupling constant									eV/m
$i$	final	Final minima	L1	L2	L3	L4	L5	L6	L7	L8	-

Table 332 Parameters of intervalley L to L optical phonon scattering

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opl[1, 2, 3, 4, 5, 6, 7, 8]								
		Description	Default								
$E_{op}$	E	Phonon energy									eV
$D_{op}$	Cc	Coupling constant									eV/m
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]								

## Chapter 19: Gallium Arsenide Material Model

### Conduction Band Model

Table 333 Parameters of intervalley L to X optical phonon scattering

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opx[1, 2, 3, 4, 5, 6]								
		Description	Default								
$E_{\text{op}}$	E	Phonon energy	$21.85 \times 10^{-3}$								eV
$D_{\text{op}}$	Cc	Coupling constant	$3.284 \times 10^{10}$								eV/m
$i$	final	Final minima	X[1, 2, 3, 4, 5, 6]								-

Table 334 Parameters of intervalley L to  $\Gamma$  optical phonon scattering

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opg								
		Description	Default								
$E_{\text{op}}$	E	Phonon energy	$22.69 \times 10^{-3}$								eV
$D_{\text{op}}$	Cc	Coupling constant	$5.25 \times 10^{10}$								eV/m
$i$	final	Final minima	G								-

## $\Gamma$ -Valley Scattering Mechanisms

The  $\Gamma$ -minimum defines the set of scattering mechanisms listed in Table 335. By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL GaAs.conduction.C2.G.<mechanism> ADD
```

```
MATERIAL GaAs.conduction.C2.G.<mechanism> REMOVE
```

## Chapter 19: Gallium Arsenide Material Model

### Conduction Band Model

Table 335 Scattering mechanisms for  $\Gamma$ -minimum

Scattering mechanism	Mechanism name
Acoustic Phonon (elastic)	ac
Polar Optical (intra)	pop
Optical Phonon (inter)	opl1
Optical Phonon (inter)	opl2
Optical Phonon (inter)	opl3
Optical Phonon (inter)	opl4
Optical Phonon (inter)	opl5
Optical Phonon (inter)	opl6
Optical Phonon (inter)	opl7
Optical Phonon (inter)	opl8
Optical Phonon (inter)	opx1
Optical Phonon (inter)	opx2
Optical Phonon (inter)	opx3
Optical Phonon (inter)	opx4
Optical Phonon (inter)	opx5
Optical Phonon (inter)	opx6
Ionized Impurity	II
Surface Roughness	SR
Remote Coulomb	RC

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for the  $\Gamma$ -minimum, listed in [Table 337](#), have the same parameter values.

## Chapter 19: Gallium Arsenide Material Model

### Conduction Band Model

To change these parameter values, use the following input file syntax:

```
MATERIAL GaAs.conduction.C2.G.<mechanism>.<parameter> <value>
```

#### Elastic Acoustic Phonon Scattering

[Table 336](#) lists the default parameter values of intravalley elastic *longitudinal* acoustic phonon scattering.

*Table 336 Parameters of elastic longitudinal acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	ac	
		Description	Default	
$\Delta_{ac}$	D	Acoustic deformation	5.0	eV
v	v	Velocity	$3.86 \times 10^3$	m/s
i	final	Final minima	G	—

#### Polar-Optical Phonon Scattering

[Table 337](#) lists the default parameter values of intravalley polar-optical phonon scattering.

*Table 337 Parameters of polar-optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	pop	
		Description	Default	
$E_{op}$	E	Phonon energy	$37.798 \times 10^{-3}$	eV
i	final	Final minima	G	—

## Chapter 19: Gallium Arsenide Material Model

Conduction Band Model

### Optical Phonon Scattering

[Table 338](#) and [Table 339](#) list the default parameter values of intervalley optical phonon scattering.

*Table 338 Parameters of intervalley  $\Gamma$  to L optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
<b>Mechanism name:</b>				<b>opl[1, 2, 3, 4, 5, 6, 7, 8]</b>
<b>Description</b>				<b>Default</b>
$E_{\text{op}}$	E	Phonon energy	$22.69 \times 10^{-3}$	eV
$D_{\text{op}}$	Cc	Coupling constant	$5.25 \times 10^{10}$	eV/m
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]	—

*Table 339 Parameters of intervalley  $\Gamma$  to X optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
<b>Mechanism name:</b>				<b>opx[1, 2, 3, 4, 5, 6]</b>
<b>Description</b>				<b>Default</b>
$E_{\text{op}}$	E	Phonon energy	$23.45 \times 10^{-3}$	eV
$D_{\text{op}}$	Cc	Coupling constant	$2.454 \times 10^{11}$	eV/m
$i$	final	Final minima	X[1, 2, 3, 4, 5, 6]	—

---

## Ionized Impurity Scattering

Ionized impurity scattering is defined for each valley in a conduction band and is treated as an intravalley process by default, so that the final valley after scattering is the same as the initial valley.

*Table 340 Parameters of ionized impurity scattering*

Parameter symbol	Parameter name	Valley name:	All valleys	Unit
		Mechanism name:	II	
		Description	Default	
<i>i</i>	final	Final minimum	Same as initial minimum	–

## Ionized Impurity Empirical Rate Factor

The ionized impurity scattering model includes a scaling factor for the empirical correction of the calculated scattering rate as a function of doping density.

To redefine the default empirical factor, use the following input file syntax:

```
MATERIAL GaAs.conduction.IIfac N <Nvalue> [<Nvalue2>] <rule> <value>
```

Here, **IIfac** is a piecewise interpolation parameter that defines a correction factor **<value>** for a value **<Nvalue>** of the doping concentration **N**. The interpolation model used to return values between specified densities is given by **<rule>**, which might require an upper bound of the density [**<Nvalue2>**]. For a description of the interpolation parameter type, see [Interpolation Methods on page 301](#).

By default, the empirical correction for ionized impurity is 1.0. However, for electrons in GaAs, a non-unity default value is provided to best match experimental low-field concentration-dependent mobility.

---

## Surface Roughness Scattering

[Table 341](#) lists the default parameter values of surface roughness scattering. These parameters apply to all valleys and to all equivalent surface orientations.

*Table 341 Parameters of surface roughness scattering*

Parameter symbol	Parameter name	Mechanism name:	SR		Unit
		Description	Default		
$\Delta$	rms	RMS amplitude	1.2	1.2	nm
$L_c$	l	Correlation length	1.0	1.0	nm
$\langle hkl \rangle$	orient	Surface orientation	(001)	(110)	–
$i$	carrier	Carrier type	electrons	electrons	–

---

## Remote Coulomb Scattering

[Table 342](#) lists the default parameter values of remote Coulomb scattering, which is treated as an intravalley process. These parameters apply to all valleys.

*Table 342 Parameters of remote Coulomb scattering*

Parameter symbol	Parameter name	Mechanism name:	RC		Unit
		Description	Default		
$z_d$	zd	Depth of charge centroid	1.5		nm
$E_0$	e0	Minimum energy for tabulating rate	0		eV
$N_0$	n0	Minimum screening density	$5 \times 10^{15}$		$\text{cm}^{-3}$
$i$	final	Final minimum	Same as initial minimum		–

---

To define the interface charge density for remote Coulomb scattering, follow the descriptions in [Defining Interface Models on page 217](#). By default, no interface charge is applied.

## Chapter 19: Gallium Arsenide Material Model

### Valence Band Model

## Valence Band Model

This section describes the valence band model.

### Band Edge Parameters

To change the default parameter values of the valence band container model, listed in [Table 343](#), use the following input file syntax:

```
MATERIAL GaAs.valence.<parameter> <value>
```

*Table 343 Parameters of valence band container model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Valence band energy with respect to vacuum	5.494	eV
$m_{dg_x}$	$dgx$	Hole density gradient effective x-mass	0.5	$m_e$
$m_{dg_y}$	$dgy$	Hole density gradient effective y-mass	0.5	$m_e$
$m_{dg_z}$	$dgz$	Hole density gradient effective z-mass	0.5	$m_e$
<b>k-p band structure model parameters</b>				
$L$	$L-kp$	Valence band parameter	0.0	$\hbar^2/2m$
$M$	$M-kp$	Valence band parameter	0.0	$\hbar^2/2m$
$N$	$N-kp$	Valence band parameter	0.0	$\hbar^2/2m$
$l$	$l-defpot$	Valence deformation potential	0.0	eV
$m$	$m-defpot$	Valence deformation potential	0.0	eV
$n$	$n-defpot$	Valence deformation potential	0.0	eV
$\Delta_{sso}$	$dsso$	Spin-orbit split energy	0.0	eV

## Chapter 19: Gallium Arsenide Material Model

### Valence Band Model

To change the default parameter values of the valence bands in the container model, listed in [Table 344](#), use the following input file syntax:

```
MATERIAL GaAs.valence.<band>.<parameter> <value>
```

*Table 344 Parameters of valence band model*

Parameter symbol	Parameter name	Description	Default	Unit
<b>Heavy hole (HH) band</b>				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.0	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	6kp	—
<b>Light hole (LH) band</b>				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.0	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	6kp	—
<b>Spin split-off (SSO) band</b>				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.044	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	6kp	—

## Mobility Models

The valence band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models together with some phenomenological enhancement factors.

### Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 345](#), use the following input file syntax:

```
MATERIAL GaAs.valence.constant.<parameter> <value>
```

## Chapter 19: Gallium Arsenide Material Model

### Valence Band Model

Table 345 Parameters of constant mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	491.5	$\text{cm}^2/\text{Vs}$
$\zeta$	zeta	Fitting parameter	2.2	—

## Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 346](#), use the following input file syntax:

```
MATERIAL GaAs.valence.Arora.<parameter> <value>
```

Table 346 Parameters of Arora mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min}$	mumin	Minimum mobility	54.3	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	491.5	$\text{cm}^2/\text{Vs}$
$N_0$	n0	Reference concentration	$2.35 \times 10^{17}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.88	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.33	—
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

## Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 347](#), use the following input file syntax:

```
MATERIAL GaAs.valence.Masetti.<parameter> <value>
```

## Chapter 19: Gallium Arsenide Material Model

### Valence Band Model

*Table 347 Parameters of Masetti mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min 1}$	mumin1	Minimum mobility	75.0	$\text{cm}^2/\text{Vs}$
$\mu_{\min 2}$	mumin2	Minimum mobility	75.0	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	491.5	$\text{cm}^2/\text{Vs}$
$\mu_1$	mul	Maximum mobility	1.0	$\text{cm}^2/\text{Vs}$
$C_r$	cr	Reference concentration	$1.0 \times 10^{18}$	$\text{cm}^{-3}$
$C_s$	cs	Reference solid solubility concentration	1.0	$\text{cm}^{-3}$
$p_c$	pc	Reference concentration	0.0	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	2.37	—
$\beta$	beta	Fitting parameter	2.0	—
$\zeta$	zeta	Fitting parameter	2.2	—

## Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 348](#), use the following input file syntax:

```
MATERIAL GaAs.valence.Yamaguchi.<parameter> <value>
```

*Table 348 Parameters of Yamaguchi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

## Chapter 19: Gallium Arsenide Material Model

### Valence Band Model

## Perpendicular Field: Lombardi Mobility Model

To change the default parameter values of the Lombardi mobility model, listed in [Table 349](#), use the following input file syntax:

```
MATERIAL GaAs.valence.Lombardi.<parameter> <value>
```

*Table 349 Parameters of Lombardi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
A	a	Fitting parameter	2.0	—
B	b	Fitting parameter	$9.925 \times 10^6$	cm/s
C	c	Fitting parameter	$2.947 \times 10^3$	$\text{cm}^{5/3} \text{V}^{-2/3} \text{s}^{-1}$
$\alpha$	alpha	Fitting parameter	0.0	$\text{cm}^3$
$\delta$	delta	Fitting parameter	$2.0546 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$2.0546 \times 10^{30}$	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	1.0	—
$\lambda$	lambda	Fitting parameter	0.0317	—
$\nu$	nu	Fitting parameter	1.0	—
$N_0$	n0	Fitting parameter	1.0	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	1.0	$\text{cm}^{-3}$
$l_{\text{crit}}$	lcrit	Critical length	$1 \times 10^{-6}$	cm

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in [Table 350](#), use the following input file syntax:

```
MATERIAL GaAs.valence.Caughey.<parameter> <value>
```

## Chapter 19: Gallium Arsenide Material Model

### Valence Band Model

Table 350 Parameters of Caughey–Thomas mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$4.5 \times 10^6$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	0.52	—
$\beta_0$	beta0	Fitting parameter	1.213	—
$\beta_{\text{exp}}$	bexp	Fitting parameter	0.17	—
$\alpha$	alpha	Fitting parameter	0.0	—

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 351](#). To change the default mobility model, use the following input file syntax:

```
MATERIAL GaAs.valence.mobility.<model> <value>
```

Table 351 Parameters of default mobility model

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley valence band model consists of the valley minima listed in [Table 352](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL GaAs.valence.<band>.<valley> REMOVE
```

### Note:

The valence band analytic valley approximation is used only as a way to define density-of-states for drift-diffusion simulations and to define the valley minima in response to stress.

## Chapter 19: Gallium Arsenide Material Model

### Valence Band Model

Table 352 Names of valence band minima

Valence band minima	Band name	Valley name
Heavy hole	HH	vhh
Light hole	LH	vlh
Spin split-off	SSO	vsso

## Position and Orientation

The position and orientation of the HH, LH, and SSO valley minima are identical. [Table 353](#) shows the default values. To change the default values, use the following input file syntax:

```
MATERIAL GaAs.valence.<band>.<valley>.min.<parameter> <value>
```

Table 353 Position and orientation parameters of HH, LH, and SSO valley minima

Parameter symbol	Parameter name	Description	Default	Unit
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.0	$2\pi/a$
x	x	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
y	y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
z	z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$

## Parameters

To change the valley minima model parameters, listed in [Table 354](#), for each valley listed in [Table 352](#), use the following input file syntax:

```
MATERIAL GaAs.valence.<band>.<valley>.<parameter> <value>
```

Table 354 Parameters of valence band minima

Parameter symbol	Parameter name	Description	Default	Unit
<b>Heavy hole (HH) band</b>				
E	E	Minima with respect to band edge	0.0	eV

## Chapter 19: Gallium Arsenide Material Model

### Valence Band Model

Table 354 Parameters of valence band minima (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$m_x$	mx	Longitudinal effective mass	0.51	$m_e$
$m_y$	my	Transverse effective mass	0.51	$m_e$
$m_z$	mz	Transverse effective mass	0.51	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	0.0	eV
<b>Light hole (LH) band</b>				
$E$	E	Minima with respect to band edge	0.0	eV
$m_x$	mx	Longitudinal effective mass	0.082	$m_e$
$m_y$	my	Transverse effective mass	0.082	$m_e$
$m_z$	mz	Transverse effective mass	0.082	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	0.0	eV
<b>Spin split-off (SSO) band</b>				
$E$	E	Minima with respect to band edge	0.341	eV
$m_x$	mx	Longitudinal effective mass	0.172	$m_e$
$m_y$	my	Transverse effective mass	0.172	$m_e$
$m_z$	mz	Transverse effective mass	0.172	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	0.0	eV

## **Heavy-Hole Band Scattering Mechanisms**

There are no heavy-hole band scattering mechanisms defined in the current version of Garand.

---

## **Light-Hole Band Scattering Mechanisms**

There are no light-hole band scattering mechanisms defined in the current version of Garand.

---

## **Spin Split-Off Band Scattering Mechanisms**

There are no spin split-off band scattering mechanisms defined in the current version of Garand.

## Indium Arsenide Material Model

---

*This chapter describes the InAs material model.*

---

### Bulk Material Model

This section describes the bulk material model for InAs.

---

#### Parameters of Bulk Material Model

To change the default parameter values in [Table 355](#), use the following input file syntax:

```
MATERIAL InAs.<parameter> <value>
```

*Table 355 Bulk material model parameters*

Parameter symbol	Parameter name	Description	Default	Unit
<b>Crystal lattice and orientation in simulation domain</b>				
a	a	Magnitude of lattice vector a	6.0583	Å
b	b	Magnitude of lattice vector b	6.0583	Å
c	c	Magnitude of lattice vector c	6.0583	Å
$\alpha$	alpha	Angle between b and c	90	degree
$\beta$	beta	Angle between c and a	90	degree
$\gamma$	gamma	Angle between a and b	90	degree
$\langle hkl \rangle_x$	x	Orientation in the x-direction	1 0 0	—

## Chapter 20: Indium Arsenide Material Model

### Bulk Material Model

Table 355 Bulk material model parameters (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$\langle hkl \rangle_z$	z	Orientation in the z-direction	0 0 1	—
<b>Bulk electrical and mechanical properties</b>				
$\kappa$	permittivity	Relative dielectric constant	15.15	—
$\kappa_\infty$	k_inf	High-frequency permittivity	12.30	—
$\rho$	density	Mass density	5.68	g/cm <sup>3</sup>
$C_{11}$	c11	Elastic stiffness matrix element	83.4	GPa
$C_{12}$	c12	Elastic stiffness matrix element	45.4	GPa
$C_{44}$	c44	Elastic stiffness matrix element	39.5	GPa

## Band-to-Band Tunneling Parameters

To change the default parameter values for the Kane model, listed in [Table 356](#), use the following input file syntax:

```
MATERIAL InAs.BTBT.<parameter> <value>
```

Table 356 Band-to-band tunneling parameters

Parameter symbol	Parameter name	Description	Default	Unit
$D_{TA}$	DTA	Acoustic phonon deformation potential	0.0	eV
$\epsilon_{TA}$	epsilonTA	Acoustic phonon energy	0.0	eV

## Chapter 20: Indium Arsenide Material Model

### Conduction Band Model

---

## Conduction Band Model

This section describes the conduction band model.

---

### Band Edge Parameters

To change the default parameter values of the conduction band container model, listed in [Table 357](#), use the following input file syntax:

```
MATERIAL InAs.conduction.<parameter> <value>
```

*Table 357 Parameters of conduction band container model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Conduction band energy with respect to vacuum	4.9	eV
$m_{dg_x}$	$dgx$	Electron density gradient effective x-mass	0.3	$m_e$
$m_{dg_y}$	$dgy$	Electron density gradient effective y-mass	0.3	$m_e$
$m_{dg_z}$	$dgz$	Electron density gradient effective z-mass	0.3	$m_e$

To change the default parameter values of the conduction bands in the container model, listed in [Table 358](#), use the following input file syntax:

```
MATERIAL InAs.conduction.<band>.<parameter> <value>
```

*Table 358 Parameters of conduction band model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Conduction band energy with respect to container energy	0.0	eV
$model$	$model$	Model used for transport in this band	ema	—

---

## Mobility Models

The conduction band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models.

### Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 359](#), use the following input file syntax:

```
MATERIAL InAs.conduction.constant.<parameter> <value>
```

*Table 359 Parameters of constant mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	$3.4 \times 10^4$	$\text{cm}^2/\text{Vs}$
$\zeta$	zeta	Fitting parameter	1.57	—

### Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 360](#), use the following input file syntax:

```
MATERIAL InAs.conduction.Arora.<parameter> <value>
```

*Table 360 Parameters of Arora mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min}$	mumin	Minimum mobility	88.0	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	$3.4 \times 10^4$	$\text{cm}^2/\text{Vs}$
$N_0$	n0	Reference concentration	$1.25 \times 10^{17}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.88	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.33	—

## Chapter 20: Indium Arsenide Material Model

### Conduction Band Model

Table 360 Parameters of Arora mobility model (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

## Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 361](#), use the following input file syntax:

```
MATERIAL InAs.conduction.Masetti.<parameter> <value>
```

Table 361 Parameters of Masetti mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min 1}$	mumin1	Minimum mobility	220.0	$\text{cm}^2/\text{Vs}$
$\mu_{\min 2}$	mumin2	Minimum mobility	220.0	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	$3.4 \times 10^4$	$\text{cm}^2/\text{Vs}$
$\mu_1$	mul	Maximum mobility	1.0	$\text{cm}^2/\text{Vs}$
$C_r$	cr	Reference concentration	$1.2 \times 10^{17}$	$\text{cm}^{-3}$
$C_s$	cs	Reference solid solubility concentration	0.0	$\text{cm}^{-3}$
$p_c$	pc	Reference concentration	0.0	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.5	—
$\beta$	beta	Fitting parameter	2.0	—
$\zeta$	zeta	Fitting parameter	1.57	—

## Chapter 20: Indium Arsenide Material Model

### Conduction Band Model

## Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 362](#), use the following input file syntax:

```
MATERIAL InAs.conduction.Yamaguchi.<parameter> <value>
```

*Table 362 Parameters of Yamaguchi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

## Perpendicular Field: Lombardi Mobility Model

To change the default parameter values of the Lombardi mobility model, listed in [Table 363](#), use the following input file syntax:

```
MATERIAL InAs.conduction.Lombardi.<parameter> <value>
```

*Table 363 Parameters of Lombardi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$A$	a	Fitting parameter	2.0	—
$B$	b	Fitting parameter	$4.75 \times 10^7$	cm/s
$C$	c	Fitting parameter	$5.80 \times 10^2$	$\text{cm}^{5/3} \text{V}^{-2/3} \text{s}^{-1}$
$\alpha$	alpha	Fitting parameter	0.0	$\text{cm}^3$
$\delta$	delta	Fitting parameter	$5.82 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$5.82 \times 10^{30}$	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	1.0	—
$\lambda$	lambda	Fitting parameter	0.125	—
$\nu$	nu	Fitting parameter	1.0	—

## Chapter 20: Indium Arsenide Material Model

### Conduction Band Model

Table 363 Parameters of Lombardi mobility model (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$N_0$	n0	Fitting parameter	1.0	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	1.0	$\text{cm}^{-3}$
$l_{\text{crit}}$	lcrit	Critical length	$1 \times 10^{-6}$	cm

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in [Table 364](#), use the following input file syntax:

```
MATERIAL InAs.conduction.Caughey.<parameter> <value>
```

Table 364 Parameters of Caughey–Thomas mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$6.0 \times 10^6$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	0.87	–
$\beta_0$	beta0	Fitting parameter	1.109	–
$\beta_{\text{exp}}$	bexp	Fitting parameter	0.66	–
$\alpha$	alpha	Fitting parameter	0.0	–

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 365](#). To change the default mobility model, use the following input file syntax:

```
MATERIAL InAs.conduction.mobility.<model> <value>
```

## Chapter 20: Indium Arsenide Material Model

### Conduction Band Model

Table 365 Parameters of default mobility model

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley conduction band model consists of the valley minima listed in [Table 366](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL InAs.conduction.<band>.<valley> REMOVE
```

Table 366 Names of conduction band C1 minima

Conduction band minimum	Valley name
X	X1, X2, X3, X4, X5, X6
L	L1, L2, L3, L4, L5, L6, L7, L8
$\Gamma$	G

## Position and Orientation

Valley minima differ in their position and orientation, the default values of which are shown in [Table 367](#), [Table 368](#), and [Table 369](#).

To change default values, use the following input file syntax:

```
MATERIAL InAs.conduction.C1.<valley>.min.<parameter> <value>
```

Table 367 Position and orientation parameters of X-minima of conduction band

Parameter symbol	Parameter name	Description	Default	Unit
X1				

$k_0$	pos	Position within the Brillouin zone	1.0 0.0 0.0	$2\pi/a$
-------	-----	------------------------------------	-------------	----------

## Chapter 20: Indium Arsenide Material Model

### Conduction Band Model

*Table 367 Position and orientation parameters of X-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$x$	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X2</b>				
$k_0$	pos	Position within the Brillouin zone	-1.0 0.0 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X3</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 1.0 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	0 1 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X4</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 -1.0 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	0 1 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X5</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 1.0	$2\pi/a$

## Chapter 20: Indium Arsenide Material Model

### Conduction Band Model

*Table 367 Position and orientation parameters of X-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
x	X	Orientation of the x-axis	0 0 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	0 -1 0	$\langle hkl \rangle$
<b>X6</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 -1.0	$2\pi/a$
x	X	Orientation of the x-axis	0 0 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	0 -1 0	$\langle hkl \rangle$

*Table 368 Position and orientation parameters of L-minima of conduction band*

Parameter symbol	Parameter name	Description	Default	Unit
<b>L1</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 1 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L2</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 1 1	$\langle hkl \rangle$

## Chapter 20: Indium Arsenide Material Model

### Conduction Band Model

*Table 368 Position and orientation parameters of L-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
y	Y	Orientation of the y-axis	1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 1 0	$\langle hkl \rangle$
<b>L3</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 -0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 -1 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$
<b>L4</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	1 1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L5</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 -0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 -1 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 -1 -2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L6</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 1 -1	$\langle hkl \rangle$

## Chapter 20: Indium Arsenide Material Model

### Conduction Band Model

*Table 368 Position and orientation parameters of L-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
y	Y	Orientation of the y-axis	1 -1 -2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$
<b>L7</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 -0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 -1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$
<b>L8</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 -0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 -1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 1 0	$\langle hkl \rangle$

*Table 369 Position and orientation parameters of  $\Gamma$ -minimum of conduction band*

Parameter symbol	Parameter name	Description	Default	Unit
<b>G</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.0	$2\pi/a$
x	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$

## Chapter 20: Indium Arsenide Material Model

### Conduction Band Model

## Parameters

To change the default parameter values of the valley minima models, listed in the following tables, for each valley listed in [Table 366](#), use the following input file syntax:

```
MATERIAL InAs.conduction.C1.<valley>.<parameter> <value>
```

### Note:

By default, all  $X$ -minima have the same parameter values, and all  $L$ -minima have the same parameter values.

*Table 370 Parameters of X-valley model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Minima with respect to band edge	1.02	eV
$m_x$	$mx$	Longitudinal effective mass	1.13	$m_e$
$m_y$	$my$	Transverse effective mass	0.16	$m_e$
$m_z$	$mz$	Transverse effective mass	0.16	$m_e$
$\alpha$	$a$	Valley nonparabolicity factor	0.9	—
$\Xi_u$	$xi\_u$	Uniaxial deformation potential	0.0	eV
$\Xi_d$	$xi\_d$	Dilatation deformation potential	0.0	eV
$\Xi'_u$	$xi\_u\_prime$	Uniaxial mass deformation	0.0	eV

*Table 371 Parameters of L-valley model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Minima with respect to band edge	0.75	eV
$m_x$	$mx$	Longitudinal effective mass	0.64	$m_e$
$m_y$	$my$	Transverse effective mass	0.05	$m_e$

## Chapter 20: Indium Arsenide Material Model

### Conduction Band Model

Table 371 Parameters of  $L$ -valley model (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$m_z$	mz	Transverse effective mass	0.05	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.45	—
$\Xi_u$	xi_u	Uniaxial deformation potential	0.0	eV
$\Xi_d$	xi_d	Dilatation deformation potential	0.0	eV
$\Xi'_u$	xi_u_prime	Uniaxial mass deformation	0.0	eV

Table 372 Parameters of  $\Gamma$ -valley model

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Minima with respect to band edge	0.0	eV
$m_x$	mx	Longitudinal effective mass	0.023	$m_e$
$m_y$	my	Transverse effective mass	0.023	$m_e$
$m_z$	mz	Transverse effective mass	0.023	$m_e$
$\alpha$	a	Valley nonparabolicity factor	2.2	—
$\Xi_u$	xi_u	Uniaxial deformation potential	0.0	eV
$\Xi_d$	xi_d	Dilatation deformation potential	0.0	eV
$\Xi'_u$	xi_u_prime	Uniaxial mass deformation	0.0	eV

## Chapter 20: Indium Arsenide Material Model

### Conduction Band Model

---

## X-Valley Scattering Mechanisms

The six *X*-minima define the set of scattering mechanisms listed in [Table 373](#). By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL InAs.conduction.C1.<valley>.<mechanism> ADD
```

```
MATERIAL InAs.conduction.C1.<valley>.<mechanism> REMOVE
```

*Table 373 Scattering mechanisms for X-minima*

Scattering mechanism	X1	X2	X3	X4	X5	X6
	Mechanism name					
Acoustic Phonon (elastic)	ac	ac	ac	ac	ac	ac
Polar Optical (intra)	pop	pop	pop	pop	pop	pop
Optical Phonon (inter)	opx2	opx1	opx1	opx1	opx1	opx1
Optical Phonon (inter)	opx3	opx3	opx2	opx3	opx3	opx3
Optical Phonon (inter)	opx4	opx4	opx4	opx2	opx4	opx4
Optical Phonon (inter)	opx5	opx5	opx5	opx5	opx2	opx5
Optical Phonon (inter)	opx6	opx6	opx6	opx6	opx6	opx2
Optical Phonon (inter)	opl1	opl1	opl1	opl1	opl1	opl1
Optical Phonon (inter)	opl2	opl2	opl2	opl2	opl2	opl2
Optical Phonon (inter)	opl3	opl3	opl3	opl3	opl3	opl3
Optical Phonon (inter)	opl4	opl4	opl4	opl4	opl4	opl4
Optical Phonon (inter)	opl5	opl5	opl5	opl5	opl5	opl5
Optical Phonon (inter)	opl6	opl6	opl6	opl6	opl6	opl6
Optical Phonon (inter)	opl7	opl7	opl7	opl7	opl7	opl7
Optical Phonon (inter)	opl8	opl8	opl8	opl8	opl8	opl8

## Chapter 20: Indium Arsenide Material Model

### Conduction Band Model

Table 373 Scattering mechanisms for X-minima (Continued)

Scattering mechanism	X1	X2	X3	X4	X5	X6
Mechanism name						
Optical Phonon (inter)	opg	opg	opg	opg	opg	opg
Ionized Impurity	II	II	II	II	II	II
Surface Roughness	SR	SR	SR	SR	SR	SR
Remote Coulomb	RC	RC	RC	RC	RC	RC

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each X-minimum, listed in [Table 373](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL InAs.conduction.C1.<valley>.<mechanism>.<parameter> <value>
```

### Elastic Acoustic Phonon Scattering

[Table 374](#) lists the default parameter values of intravalley elastic acoustic phonon scattering.

Table 374 Parameters of elastic acoustic phonon scattering

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
Mechanism name: ac									
		Description	Default						
$\Delta_{ac}$	D	Acoustic deformation	5.8						eV
$v$	v	Velocity		$3.09 \times 10^3$					m/s
$i$	final	Final minima	X1	X2	X3	X4	X5	X6	-

## Chapter 20: Indium Arsenide Material Model

Conduction Band Model

### Polar-Optical Phonon Scattering

[Table 375](#) lists the default parameter values of intravalley polar-optical phonon scattering.

*Table 375 Parameters of polar-optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
<b>Mechanism name:</b> pop									
<b>Description</b>									<b>Default</b>
$E_{op}$	E	Phonon energy							eV
$i$	final	Final minima	X1	X2	X3	X4	X5	X6	—

### Optical Phonon Scattering

[Table 376](#) to [Table 378](#) list the default parameter values of intervalley optical phonon scattering.

*Table 376 Parameters of intervalley X to X optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
<b>Mechanism name:</b> opx [1, 2, 3, 4, 5, 6]									
<b>Description</b>									<b>Default</b>
$E_{op}$	E	Phonon energy							eV
$D_{op}$	Cc	Coupling constant							eV/m
$i$	final	Final minima	X[1, 2, 3, 4, 5, 6]						—

## Chapter 20: Indium Arsenide Material Model

### Conduction Band Model

*Table 377 Parameters of intervalley X to L optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
<b>Mechanism name: opl[1, 2, 3, 4, 5, 6, 7, 8]</b>									
<b>Description</b>									<b>Default</b>
$E_{op}$	E	Phonon energy							eV
$D_{op}$	Cc	Coupling constant							eV/m
$i$	final	Final minima							—

*Table 378 Parameters of intervalley X to  $\Gamma$  optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
<b>Mechanism name: opg</b>									
<b>Description</b>									<b>Default</b>
$E_{op}$	E	Phonon energy							eV
$D_{op}$	Cc	Coupling constant							eV/m
$i$	final	Final minima				G			—

## L-Valley Scattering Mechanisms

The eight L-minima define the set of scattering mechanisms listed in [Table 379](#). By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL InAs.conduction.C1.<valley>.<mechanism> ADD
```

```
MATERIAL InAs.conduction.C1.<valley>.<mechanism> REMOVE
```

## Chapter 20: Indium Arsenide Material Model

### Conduction Band Model

Table 379 Scattering mechanisms for L-minima

Scattering mechanism	L1	L2	L3	L4	L5	L6	L7	L8
	Mechanism name							
Acoustic Phonon (elastic)	ac	ac	ac	ac	ac	ac	ac	ac
Polar Optical (intra)	pop	pop	pop	pop	pop	pop	pop	pop
Optical Phonon (intra)	opl	opl	opl	opl	opl	opl	opl	opl
Optical Phonon (inter)	opl2	opl1						
Optical Phonon (inter)	opl3	opl3	opl2	opl2	opl2	opl2	opl2	opl2
Optical Phonon (inter)	opl4	opl4	opl4	opl3	opl3	opl3	opl3	opl3
Optical Phonon (inter)	opl5	opl5	opl5	opl5	opl4	opl4	opl4	opl4
Optical Phonon (inter)	opl6	opl6	opl6	opl6	opl6	opl5	opl5	opl5
Optical Phonon (inter)	opl7	opl7	opl7	opl7	opl7	opl7	opl6	opl6
Optical Phonon (inter)	opl8	opl8	opl8	opl8	opl8	opl8	opl8	opl7
Optical Phonon (inter)	opx1	opx1	opx1	opx1	opx1	opx1	opx1	opx1
Optical Phonon (inter)	opx2	opx2	opx2	opx2	opx2	opx2	opx2	opx2
Optical Phonon (inter)	opx3	opx3	opx3	opx3	opx3	opx3	opx3	opx3
Optical Phonon (inter)	opx4	opx4	opx4	opx4	opx4	opx4	opx4	opx4
Optical Phonon (inter)	opx5	opx5	opx5	opx5	opx5	opx5	opx5	opx5
Optical Phonon (inter)	opx6	opx6	opx6	opx6	opx6	opx6	opx6	opx6
Optical Phonon (inter)	opg	opg	opg	opg	opg	opg	opg	opg
Ionized Impurity	II	II	II	II	II	II	II	II
Surface Roughness	SR	SR	SR	SR	SR	SR	SR	SR
Remote Coulomb	RC	RC	RC	RC	RC	RC	RC	RC

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each  $L$ -minimum, listed in [Table 379](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL InAs.conduction.C1.<valley>.<mechanism>.<parameter> <value>
```

### Elastic Acoustic Phonon Scattering

[Table 380](#) lists the default parameter values of intravalley elastic *longitudinal* acoustic phonon scattering.

*Table 380 Parameters of elastic longitudinal acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	ac								
		Description	Default								
$\Delta_{ac}$	D	Acoustic deformation	5.8								eV
$v$	v	Velocity									m/s
$i$	final	Final minima	L1	L2	L3	L4	L5	L6	L7	L8	—

### Polar-Optical Phonon Scattering

[Table 381](#) lists the default parameter values of intravalley polar-optical phonon scattering.

*Table 381 Parameters of polar-optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	pop								
		Description	Default								
$E_{op}$	E	Phonon energy									eV
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]								—

## Chapter 20: Indium Arsenide Material Model

### Conduction Band Model

#### Optical Phonon Scattering

[Table 382](#) to [Table 385](#) list the default parameter values of intravalley and intervalley optical phonon scattering.

*Table 382 Parameters of intravalley optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opl								
		Description	Default								
$E_{\text{op}}$	E	Phonon energy	19.23	$\times 10^{-3}$							eV
$D_{\text{op}}$	Cc	Coupling constant	6.35	$\times 10^{10}$							eV/m
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]								

*Table 383 Parameters of intervalley L to L optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	opl[1, 2, 3, 4, 5, 6, 7, 8]								
		Description	Default								
$E_{\text{op}}$	E	Phonon energy	19.23	$\times 10^{-3}$							eV
$D_{\text{op}}$	Cc	Coupling constant	6.35	$\times 10^{10}$							eV/m
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]								

## Chapter 20: Indium Arsenide Material Model

### Conduction Band Model

*Table 384 Parameters of intervalley L to X optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit		
		<b>Mechanism name:</b>	<b>opx[1, 2, 3, 4, 5, 6]</b>										
		<b>Description</b>	<b>Default</b>										
$E_{\text{op}}$	E	Phonon energy									eV		
$D_{\text{op}}$	Cc	Coupling constant									eV/m		
$i$	final	Final minima									—		
			X[1, 2, 3, 4, 5, 6]										

*Table 385 Parameters of intervalley L to  $\Gamma$  optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit		
		<b>Mechanism name:</b>	<b>opg</b>										
		<b>Description</b>	<b>Default</b>										
$E_{\text{op}}$	E	Phonon energy									eV		
$D_{\text{op}}$	Cc	Coupling constant									eV/m		
$i$	final	Final minima									—		
			G										

## $\Gamma$ -Valley Scattering Mechanisms

The default  $\Gamma$ -minimum defines the set of scattering mechanisms listed in [Table 386](#). By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL InAs.conduction.C2.G.<mechanism> ADD
```

```
MATERIAL InAs.conduction.C2.G.<mechanism> REMOVE
```

**Chapter 20: Indium Arsenide Material Model**

## Conduction Band Model

*Table 386 Scattering mechanisms for  $\Gamma$ -minimum*

Scattering mechanism	Mechanism name
Acoustic Phonon (elastic)	ac
Polar Optical (intra)	pop
Optical Phonon (inter)	opl1
Optical Phonon (inter)	opl2
Optical Phonon (inter)	opl3
Optical Phonon (inter)	opl4
Optical Phonon (inter)	opl5
Optical Phonon (inter)	opl6
Optical Phonon (inter)	opl7
Optical Phonon (inter)	opl8
Optical Phonon (inter)	opx1
Optical Phonon (inter)	opx2
Optical Phonon (inter)	opx3
Optical Phonon (inter)	opx4
Optical Phonon (inter)	opx5
Optical Phonon (inter)	opx6
Ionized Impurity	II
Surface Roughness	SR
Remote Coulomb	RC

## Chapter 20: Indium Arsenide Material Model

### Conduction Band Model

## Parameters of Scattering Mechanisms

To change the default parameter values of the scattering mechanisms, listed in [Table 386](#), use the following input file syntax:

```
MATERIAL InAs.conduction.C2.G.<mechanism>.<parameter> <value>
```

### Elastic Acoustic Phonon Scattering

[Table 387](#) lists the default parameter values of intravalley elastic *longitudinal* acoustic phonon scattering.

*Table 387 Parameters of elastic longitudinal acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	ac	
		Description	Default	
$\Delta_{ac}$	D	Acoustic deformation	5.8	eV
v	v	Velocity	$3.09 \times 10^3$	m/s
i	final	Final minima	G	—

### Polar-Optical Phonon Scattering

[Table 388](#) lists the default parameter values of intravalley polar-optical phonon scattering.

*Table 388 Parameters of polar-optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	pop	
		Description	Default	
$E_{op}$	E	Phonon energy	$32.518 \times 10^{-3}$	eV
i	final	Final minima	G	—

## Chapter 20: Indium Arsenide Material Model

### Conduction Band Model

#### Optical Phonon Scattering

Table 389 and Table 390 list the default parameter values of intervalley optical phonon scattering.

Table 389 Parameters of intervalley  $\Gamma$  to L optical phonon scattering

Parameter symbol	Parameter name	Valley name:	G	Unit
Mechanism name: opl[1, 2, 3, 4, 5, 6, 7, 8]				
		Description	Default	
$E_{\text{op}}$	E	Phonon energy	$17.45 \times 10^{-3}$	eV
$D_{\text{op}}$	Cc	Coupling constant	$5.59 \times 10^{10}$	eV/m
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]	-

Table 390 Parameters of intervalley  $\Gamma$  to X optical phonon scattering

Parameter symbol	Parameter name	Valley name:	G	Unit
Mechanism name: opx[1, 2, 3, 4, 5, 6]				
		Description	Default	
$E_{\text{op}}$	E	Phonon energy	$19.23 \times 10^{-3}$	eV
$D_{\text{op}}$	Cc	Coupling constant	$25.41 \times 10^{10}$	eV/m
$i$	final	Final minima	X[1, 2, 3, 4, 5, 6]	-

---

## Ionized Impurity Scattering

Ionized impurity scattering is defined for each valley in a conduction band and is treated as an intravalley process by default, so that the final valley after scattering is the same as the initial valley.

*Table 391 Parameters of ionized impurity scattering*

Parameter symbol	Parameter name	Valley name:	All valleys	Unit
		Mechanism name:	II	
		Description	Default	
<i>i</i>	final	Final minimum	Same as initial minimum	–

## Ionized Impurity Empirical Rate Factor

The ionized impurity scattering model includes a scaling factor for the empirical correction of the calculated scattering rate as a function of doping density.

To redefine the default empirical factor, use the following input file syntax:

```
MATERIAL InAs.conduction.IIfac N <Nvalue> [<Nvalue2>] <rule> <value>
```

Here, **IIfac** is a piecewise interpolation parameter that defines a correction factor **<value>** for a value **<Nvalue>** of the doping concentration **N**. The interpolation model used to return values between specified densities is given by **<rule>**, which might require an upper bound of the density [**<Nvalue2>**]. For a description of the interpolation parameter type, see [Interpolation Methods on page 301](#).

By default, the empirical correction for ionized impurity is 1.0. However, for electrons in InAs, a non-unity default value is provided to best match experimental low-field concentration-dependent mobility.

---

## Surface Roughness Scattering

[Table 392](#) lists the default parameter values of surface roughness scattering. These parameters apply to all valleys and to all equivalent surface orientations.

Table 392 Parameters of surface roughness scattering

Parameter symbol	Parameter name	Mechanism name: SR	Unit		
		Description	Default		
$\Delta$	rms	RMS amplitude	1.2	1.2	nm
$L_c$	l	Correlation length	1.0	1.0	nm
$\langle hkl \rangle$	orient	Surface orientation	(001)	(110)	–
$i$	carrier	Carrier type	electrons	electrons	–

---

## Remote Coulomb Scattering

[Table 393](#) lists the default parameter values of remote Coulomb scattering, which is treated as an intravalley process. These parameters apply to all valleys.

Table 393 Parameters of remote Coulomb scattering

Parameter symbol	Parameter name	Mechanism name: RC	Unit	
		Description	Default	
$z_d$	zd	Depth of charge centroid	1.5	nm
$E_0$	E0	Minimum energy for tabulating rate	0	eV
$N_0$	N0	Minimum screening density	$5 \times 10^{15}$	$\text{cm}^{-3}$
$i$	final	Final minimum	Same as initial minimum	–

---

To define the interface charge density for remote Coulomb scattering, follow the descriptions in [Defining Interface Models on page 217](#). By default, no interface charge is applied.

---

## Valence Band Model

This section describes the valence band model.

---

### Band Edge Parameters

To change the default parameter values of the valence band container model, listed in [Table 394](#), use the following input file syntax:

```
MATERIAL InAs.valence.<parameter> <value>
```

*Table 394 Parameters of valence band container model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Valence band energy with respect to vacuum	5.254	eV
$m_{dg_x}$	$dgx$	Hole density gradient effective x-mass	0.5	$m_e$
$m_{dg_y}$	$dgy$	Hole density gradient effective y-mass	0.5	$m_e$
$m_{dg_z}$	$dgz$	Hole density gradient effective z-mass	0.5	$m_e$
<b>k·p band structure model parameters</b>				
$L$	$L-kp$	Valence band parameter	0.0	$\hbar^2/2m$
$M$	$M-kp$	Valence band parameter	0.0	$\hbar^2/2m$
$N$	$N-kp$	Valence band parameter	0.0	$\hbar^2/2m$
$l$	$l-defpot$	Valence deformation potential	0.0	eV
$m$	$m-defpot$	Valence deformation potential	0.0	eV
$n$	$n-defpot$	Valence deformation potential	0.0	eV
$\Delta_{sso}$	$dsso$	Spin-orbit split energy	0.0	eV

## Chapter 20: Indium Arsenide Material Model

### Valence Band Model

To change the default parameter values of the valence bands in the container model, listed in [Table 395](#), use the following input file syntax:

```
MATERIAL InAs.valence.<band>.<parameter> <value>
```

*Table 395 Parameters of valence band model*

Parameter symbol	Parameter name	Description	Default	Unit
Heavy hole (HH) band				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.0	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	6kp	—
Light hole (LH) band				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.0	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	6kp	—
Spin split-off (SSO) band				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.044	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	6kp	—

## Mobility Models

The valence band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models together with some phenomenological enhancement factors.

### Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 396](#), use the following input file syntax:

```
MATERIAL InAs.valence.constant.<parameter> <value>
```

## Chapter 20: Indium Arsenide Material Model

### Valence Band Model

Table 396 Parameters of constant mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	530	$\text{cm}^2/\text{Vs}$
$\zeta$	zeta	Fitting parameter	2.3	—

## Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 397](#), use the following input file syntax:

```
MATERIAL InAs.valence.Arora.<parameter> <value>
```

Table 397 Parameters of Arora mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min}$	mumin	Minimum mobility	54.3	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	530	$\text{cm}^2/\text{Vs}$
$N_0$	n0	Reference concentration	$2.35 \times 10^{17}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.88	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.33	—
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

## Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 398](#), use the following input file syntax:

```
MATERIAL InAs.valence.Masetti.<parameter> <value>
```

## Chapter 20: Indium Arsenide Material Model

### Valence Band Model

Table 398 Parameters of Masetti mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min 1}$	mumin1	Minimum mobility	75.0	cm <sup>2</sup> /Vs
$\mu_{\min 2}$	mumin2	Minimum mobility	75.0	cm <sup>2</sup> /Vs
$\mu_{\max}$	mumax	Maximum mobility	530	cm <sup>2</sup> /Vs
$\mu_1$	mul	Maximum mobility	10.0	cm <sup>2</sup> /Vs
$C_r$	cr	Reference concentration	$1.0 \times 10^{18}$	cm <sup>-3</sup>
$C_s$	cs	Reference solid solubility concentration	1.0	cm <sup>-3</sup>
$p_c$	pc	Reference concentration	0.0	cm <sup>-3</sup>
$\alpha$	alpha	Fitting parameter	2.37	—
$\beta$	beta	Fitting parameter	2.0	—
$\zeta$	zeta	Fitting parameter	2.3	—

## Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 399](#), use the following input file syntax:

```
MATERIAL InAs.valence.Yamaguchi.<parameter> <value>
```

Table 399 Parameters of Yamaguchi mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

## Chapter 20: Indium Arsenide Material Model

### Valence Band Model

## Perpendicular Field: Lombardi Mobility Model

To change the default parameter values of the Lombardi mobility model, listed in [Table 400](#), use the following input file syntax:

```
MATERIAL InAs.valence.Lombardi.<parameter> <value>
```

*Table 400 Parameters of Lombardi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
A	a	Fitting parameter	2.0	—
B	b	Fitting parameter	$9.925 \times 10^6$	cm/s
C	c	Fitting parameter	$2.947 \times 10^3$	$\text{cm}^{5/3} \text{V}^{-2/3} \text{s}^{-1}$
$\alpha$	alpha	Fitting parameter	0.0	$\text{cm}^3$
$\delta$	delta	Fitting parameter	$2.0546 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$2.0546 \times 10^{30}$	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	1.0	—
$\lambda$	lambda	Fitting parameter	0.0317	—
$\nu$	nu	Fitting parameter	1.0	—
$N_0$	n0	Fitting parameter	1.0	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	1.0	$\text{cm}^{-3}$
$l_{\text{crit}}$	lcrit	Critical length	$1 \times 10^{-6}$	cm

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in [Table 401](#), use the following input file syntax:

```
MATERIAL InAs.valence.Caughey.<parameter> <value>
```

## Chapter 20: Indium Arsenide Material Model

### Valence Band Model

Table 401 Parameters of Caughey–Thomas mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$4.5 \times 10^6$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	0.52	—
$\beta_0$	beta0	Fitting parameter	1.213	—
$\beta_{\text{exp}}$	bexp	Fitting parameter	0.17	—
$\alpha$	alpha	Fitting parameter	0.0	—

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 402](#). To change the default mobility model, use the following input file syntax:

```
MATERIAL InAs.valence.mobility.<model> <value>
```

Table 402 Parameters of default mobility model

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley valence band model consists of the valley minima listed in [Table 403](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL InAs.valence.<band>.<valley> REMOVE
```

### Note:

The valence band analytic valley approximation is used only as a way to define density-of-states for drift-diffusion simulations and to define the valley minima in response to stress.

## Chapter 20: Indium Arsenide Material Model

### Valence Band Model

Table 403 Names of valence band minima

Valence band minima	Band name	Valley name
Heavy hole	HH	vhh
Light hole	LH	vlh
Spin split-off	SSO	vsso

## Position and Orientation

The position and orientation of the HH, LH, and SSO valley minima are identical. [Table 404](#) shows the default values. To change the default values, use the following input file syntax:

```
MATERIAL InAs.valence.<band>.<valley>.min.<parameter> <value>
```

Table 404 Position and orientation parameters of HH, LH, SSO valley minima

Parameter symbol	Parameter name	Description	Default	Unit
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.0	$2\pi/a$
x	x	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
y	y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
z	z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$

## Parameters

To change the valley minima model parameters, listed in [Table 405](#), for each valley listed in [Table 403](#), use the following input file syntax:

```
MATERIAL InAs.valence.<band>.<valley>.<parameter> <value>
```

Table 405 Parameters of valence band minima

Parameter symbol	Parameter name	Description	Default	Unit
<b>Heavy hole (HH) band</b>				
E	E	Minima with respect to band edge	0.0	eV

## Chapter 20: Indium Arsenide Material Model

### Valence Band Model

Table 405 Parameters of valence band minima (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$m_x$	mx	Longitudinal effective mass	0.41	$m_e$
$m_y$	my	Transverse effective mass	0.41	$m_e$
$m_z$	mz	Transverse effective mass	0.41	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	0.0	eV
<b>Light hole (LH) band</b>				
$E$	E	Minima with respect to band edge	0.0	eV
$m_x$	mx	Longitudinal effective mass	0.026	$m_e$
$m_y$	my	Transverse effective mass	0.026	$m_e$
$m_z$	mz	Transverse effective mass	0.026	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	0.0	eV
<b>Spin split-off (SSO) band</b>				
$E$	E	Minima with respect to band edge	0.39	eV
$m_x$	mx	Longitudinal effective mass	0.14	$m_e$
$m_y$	my	Transverse effective mass	0.14	$m_e$
$m_z$	mz	Transverse effective mass	0.14	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	0.0	eV

## **Heavy-Hole Band Scattering Mechanisms**

There are no heavy-hole band scattering mechanisms defined in the current version of Garand.

---

## **Light-Hole Band Scattering Mechanisms**

There are no light-hole band scattering mechanisms defined in the current version of Garand.

---

## **Spin Split-Off Band Scattering Mechanisms**

There are no spin split-off band scattering mechanisms defined in the current version of Garand.

## Aluminum Arsenide Material Model

---

*This chapter describes the AlAs material model.*

---

### Bulk Material Model

This section describes the bulk material model for AlAs.

---

#### Parameters of Bulk Material Model

To change the default parameter values in [Table 406](#), use the following input file syntax:

```
MATERIAL AlAs.<parameter> <value>
```

*Table 406 Bulk material model parameters*

Parameter symbol	Parameter name	Description	Default	Unit
<b>Crystal lattice and orientation in simulation domain</b>				
a	a	Magnitude of lattice vector a	5.6611	Å
b	b	Magnitude of lattice vector b	5.6611	Å
c	c	Magnitude of lattice vector c	5.6611	Å
$\alpha$	alpha	Angle between b and c	90	degree
$\beta$	beta	Angle between c and a	90	degree
$\gamma$	gamma	Angle between a and b	90	degree
$\langle hkl \rangle_x$	x	Orientation in the x-direction	1 0 0	—

**Chapter 21: Aluminum Arsenide Material Model**  
 Bulk Material Model

*Table 406 Bulk material model parameters (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$\langle hkl \rangle_z$	z	Orientation in the z-direction	0 0 1	–
<b>Bulk electrical and mechanical properties</b>				
$\kappa$	permittivity	Relative dielectric constant	10.06	–
$\kappa_\infty$	k_inf	High-frequency permittivity	8.16	–
$\rho$	density	Mass density	3.76	g/cm <sup>3</sup>
$C_{11}$	C11	Elastic stiffness matrix element	120.2	GPa
$C_{12}$	C12	Elastic stiffness matrix element	57.0	GPa
$C_{44}$	C44	Elastic stiffness matrix element	59.9	GPa

## Band-to-Band Tunneling Parameters

To change the default parameter values for the Kane model, listed in [Table 407](#), use the following input file syntax:

```
MATERIAL AlAs.BTBT.<parameter> <value>
```

*Table 407 Band-to-band tunneling parameters*

Parameter symbol	Parameter name	Description	Default	Unit
$D_{TA}$	DTA	Acoustic phonon deformation potential	0.0	eV
$\epsilon_{TA}$	epsilonTA	Acoustic phonon energy	0.0	eV

## Chapter 21: Aluminum Arsenide Material Model

### Conduction Band Model

---

## Conduction Band Model

This section describes the conduction band model.

---

### Band Edge Parameters

To change the default parameter values of the conduction band container model, listed in [Table 408](#), use the following input file syntax:

```
MATERIAL AlAs.conduction.<parameter> <value>
```

*Table 408 Parameters of conduction band container model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Conduction band energy with respect to vacuum	3.5	eV
$m_{dg_x}$	$dgx$	Electron density gradient effective x-mass	0.3	$m_e$
$m_{dg_y}$	$dgy$	Electron density gradient effective y-mass	0.3	$m_e$
$m_{dg_z}$	$dgz$	Electron density gradient effective z-mass	0.3	$m_e$

To change the default parameter values of the conduction bands in the container model, listed in [Table 409](#), use the following input file syntax:

```
MATERIAL AlAs.conduction.<band>.<parameter> <value>
```

*Table 409 Parameters of conduction band model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Conduction band energy with respect to container energy	0.0	eV
$model$	$model$	Model used for transport in this band	ema	—

## Mobility Models

The conduction band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models.

### Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 410](#), use the following input file syntax:

```
MATERIAL AlAs.conduction.constant.<parameter> <value>
```

*Table 410 Parameters of constant mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	$2.5 \times 10^3$	$\text{cm}^2/\text{Vs}$
$\zeta$	zeta	Fitting parameter	1	—

### Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 411](#), use the following input file syntax:

```
MATERIAL AlAs.conduction.Arora.<parameter> <value>
```

*Table 411 Parameters of Arora mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min}$	mumin	Minimum mobility	88.0	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	$2.5 \times 10^3$	$\text{cm}^2/\text{Vs}$
$N_0$	n0	Reference concentration	$1.25 \times 10^{17}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.88	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.33	—

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*Table 411 Parameters of Arora mobility model (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

## Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 412](#), use the following input file syntax:

```
MATERIAL AlAs.conduction.Masetti.<parameter> <value>
```

*Table 412 Parameters of Masetti mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min 1}$	mumin1	Minimum mobility	220.0	$\text{cm}^2/\text{Vs}$
$\mu_{\min 2}$	mumin2	Minimum mobility	220.0	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	$2.5 \times 10^3$	$\text{cm}^2/\text{Vs}$
$\mu_1$	mul	Maximum mobility	1.0	$\text{cm}^2/\text{Vs}$
$C_r$	cr	Reference concentration	$1.2 \times 10^{17}$	$\text{cm}^{-3}$
$C_s$	cs	Reference solid solubility concentration	0.0	$\text{cm}^{-3}$
$p_c$	pc	Fitting parameter	0.0	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.5	—
$\beta$	beta	Fitting parameter	2.0	—
$\zeta$	zeta	Fitting parameter	1	—

## Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 413](#), use the following input file syntax:

```
MATERIAL AlAs.conduction.Yamaguchi.<parameter> <value>
```

*Table 413 Parameters of Yamaguchi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

## Perpendicular Field: Lombardi Mobility Model

To change the default parameter values of the Lombardi mobility model, listed in [Table 414](#), use the following input file syntax:

```
MATERIAL AlAs.conduction.Lombardi.<parameter> <value>
```

*Table 414 Parameters of Lombardi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$A$	a	Fitting parameter	2.0	—
$B$	b	Fitting parameter	$4.75 \times 10^7$	cm/s
$C$	c	Fitting parameter	$5.80 \times 10^2$	$\text{cm}^{5/3} \text{V}^{-2/3} \text{s}^{-1}$
$\alpha$	alpha	Fitting parameter	0.0	$\text{cm}^3$
$\delta$	delta	Fitting parameter	$7.02 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$5.82 \times 10^{30}$	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	1.0	—
$\lambda$	lambda	Fitting parameter	0.125	—
$\nu$	nu	Fitting parameter	1.0	—

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*Table 414 Parameters of Lombardi mobility model (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$N_0$	n0	Fitting parameter	1.0	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	1.0	$\text{cm}^{-3}$
$l_{\text{crit}}$	lcrit	Critical length	$1 \times 10^{-6}$	cm

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in [Table 415](#), use the following input file syntax:

```
MATERIAL AlAs.conduction.Caughey.<parameter> <value>
```

*Table 415 Parameters of Caughey–Thomas mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$6.0 \times 10^6$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	0.87	—
$\beta_0$	beta0	Fitting parameter	1.109	—
$\beta_{\text{exp}}$	bexp	Fitting parameter	0.66	—
$\alpha$	alpha	Fitting parameter	0.0	—

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 416](#). To change the default mobility model, use the following input file syntax:

```
MATERIAL AlAs.conduction.mobility.<model> <value>
```

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*Table 416 Parameters of default mobility model*

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley conduction band model consists of the valley minima listed in [Table 417](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL AlAs.conduction.<band>.<valley> REMOVE
```

*Table 417 Names of conduction band C1 minima*

Conduction band minimum	Valley name
X	X1, X2, X3, X4, X5, X6
L	L1, L2, L3, L4, L5, L6, L7, L8
$\Gamma$	G

## Position and Orientation

Valley minima differ in their position and orientation, the default values of which are presented in [Table 418](#), [Table 419](#), and [Table 420](#).

To change default values, use the following input file syntax:

```
MATERIAL AlAs.conduction.C1.<valley>.min.<parameter> <value>
```

*Table 418 Position and orientation parameters of X-minima of conduction band*

Parameter symbol	Parameter name	Description	Default	Unit
X1				
$k_0$	pos	Position within the Brillouin zone	1.0 0.0 0.0	$2\pi/a$

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*Table 418 Position and orientation parameters of X-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$x$	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X2</b>				
$k_0$	pos	Position within the Brillouin zone	-1.0 0.0 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X3</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 1.0 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	0 1 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X4</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 -1.0 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	0 1 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X5</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 1.0	$2\pi/a$

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*Table 418 Position and orientation parameters of X-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
x	X	Orientation of the x-axis	0 0 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	0 -1 0	$\langle hkl \rangle$
<b>X6</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 -1.0	$2\pi/a$
x	X	Orientation of the x-axis	0 0 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	0 -1 0	$\langle hkl \rangle$

*Table 419 Position and orientation parameters of L-minima of conduction band*

Parameter symbol	Parameter name	Description	Default	Unit
<b>L1</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 1 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L2</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 1 1	$\langle hkl \rangle$

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*Table 419 Position and orientation parameters of L-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
y	Y	Orientation of the y-axis	1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 1 0	$\langle hkl \rangle$
<b>L3</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 -0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 -1 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$
<b>L4</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	1 1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L5</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 -0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 -1 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 -1 -2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L6</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 1 -1	$\langle hkl \rangle$

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### Conduction Band Model

*Table 419 Position and orientation parameters of L-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
y	Y	Orientation of the y-axis	1 -1 -2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$
<b>L7</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 -0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 -1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$
<b>L8</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 -0.5 -0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 -1 -1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 1 0	$\langle hkl \rangle$

*Table 420 Position and orientation parameters of  $\Gamma$ -minimum of conduction band*

Parameter symbol	Parameter name	Description	Default	Unit
<b>G</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.0	$2\pi/a$
x	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$

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### Conduction Band Model

## Parameters

To change the default parameter values of the valley minima models, listed in the following tables, for each valley listed in [Table 421](#), use the following input file syntax:

```
MATERIAL AlAs.conduction.C1.<valley>.<parameter> <value>
```

### Note:

By default, all  $X$ -minima have the same parameter values, and all  $L$ -minima have the same parameter values.

*Table 421 Parameters of X-valley model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Minima with respect to band edge	0.00	eV
$m_x$	mx	Longitudinal effective mass	0.97	$m_e$
$m_y$	my	Transverse effective mass	0.22	$m_e$
$m_z$	mz	Transverse effective mass	0.22	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.83	—
$\Xi_u$	xi_u	Uniaxial deformation potential	0.0	eV
$\Xi_d$	xi_d	Dilatation deformation potential	0.0	eV
$\Xi'_u$	xi_u_prime	Uniaxial mass deformation	0.0	eV

*Table 422 Parameters of L-valley model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Minima with respect to band edge	0.22	eV
$m_x$	mx	Longitudinal effective mass	1.32	$m_e$

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### Conduction Band Model

Table 422 Parameters of L-valley model (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$m_y$	my	Transverse effective mass	0.15	$m_e$
$m_z$	mz	Transverse effective mass	0.15	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.45	—
$\Xi_u$	xi_u	Uniaxial deformation potential	0.0	eV
$\Xi_d$	xi_d	Dilatation deformation potential	0.0	eV
$\Xi'_u$	xi_u_prime	Uniaxial mass deformation	0.0	eV

Table 423 Parameters of  $\Gamma$ -valley model

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Minima with respect to band edge	0.859	eV
$m_x$	mx	Longitudinal effective mass	0.15	$m_e$
$m_y$	my	Transverse effective mass	0.15	$m_e$
$m_z$	mz	Transverse effective mass	0.15	$m_e$
$\alpha$	a	Valley nonparabolicity factor	1.1	—
$\Xi_u$	xi_u	Uniaxial deformation potential	0.0	eV
$\Xi_d$	xi_d	Dilatation deformation potential	0.0	eV
$\Xi'_u$	xi_u_prime	Uniaxial mass deformation	0.0	eV

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## X-Valley Scattering Mechanisms

The six *X*-minima define the set of scattering mechanisms listed in [Table 424](#). By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL AlAs.conduction.C1.<valley>.<mechanism> ADD
```

```
MATERIAL AlAs.conduction.C1.<valley>.<mechanism> REMOVE
```

*Table 424 Scattering mechanisms for X-minima*

Scattering mechanism	X1	X2	X3	X4	X5	X6
	Mechanism name					
Acoustic Phonon (elastic)	ac	ac	ac	ac	ac	ac
Polar Optical (intra)	pop	pop	pop	pop	pop	pop
Optical Phonon (inter)	opx2	opx1	opx1	opx1	opx1	opx1
Optical Phonon (inter)	opx3	opx3	opx2	opx3	opx3	opx3
Optical Phonon (inter)	opx4	opx4	opx4	opx2	opx4	opx4
Optical Phonon (inter)	opx5	opx5	opx5	opx5	opx2	opx5
Optical Phonon (inter)	opx6	opx6	opx6	opx6	opx6	opx2
Optical Phonon (inter)	opl1	opl1	opl1	opl1	opl1	opl1
Optical Phonon (inter)	opl2	opl2	opl2	opl2	opl2	opl2
Optical Phonon (inter)	opl3	opl3	opl3	opl3	opl3	opl3
Optical Phonon (inter)	opl4	opl4	opl4	opl4	opl4	opl4
Optical Phonon (inter)	opl5	opl5	opl5	opl5	opl5	opl5
Optical Phonon (inter)	opl6	opl6	opl6	opl6	opl6	opl6
Optical Phonon (inter)	opl7	opl7	opl7	opl7	opl7	opl7
Optical Phonon (inter)	opl8	opl8	opl8	opl8	opl8	opl8

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### Conduction Band Model

*Table 424 Scattering mechanisms for X-minima (Continued)*

Scattering mechanism	X1	X2	X3	X4	X5	X6
<b>Mechanism name</b>						
Optical Phonon (inter)	opg	opg	opg	opg	opg	opg
Ionized Impurity	II	II	II	II	II	II
Surface Roughness	SR	SR	SR	SR	SR	SR
Remote Coulomb	RC	RC	RC	RC	RC	RC

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each *X*-minimum, listed in [Table 424](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL AlAs.conduction.C1.<valley>.<mechanism>.<parameter> <value>
```

### Elastic Acoustic Phonon Scattering

[Table 425](#) lists the default parameter values of intravalley elastic acoustic phonon scattering.

*Table 425 Parameters of elastic acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
<b>Mechanism name:</b>									ac
<b>Description</b>									<b>Default</b>
$\Delta_{ac}$	D	Acoustic deformation	7.0						eV
$v$	v	Velocity		4.4833×10 <sup>3</sup>					m/s
$i$	final	Final minima	X1	X2	X3	X4	X5	X6	–

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### Polar-Optical Phonon Scattering

Table 426 lists the default parameter values of intravalley polar-optical phonon scattering.

Table 426 Parameters of polar-optical phonon scattering

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit		
		Mechanism name:	pop								
		Description	Default								
$E_{\text{op}}$	E	Phonon energy			$50.09 \times 10^{-3}$				eV		
$i$	final	Final minima	X1	X2	X3	X4	X5	X6	—		

### Optical Phonon Scattering

Table 427 to Table 429 list the default parameter values of intervalley optical phonon scattering.

Table 427 Parameters of intervalley X to X optical phonon scattering

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit		
		Mechanism name:	opx [1, 2, 3, 4, 5, 6]								
		Description	Default								
$E_{\text{op}}$	E	Phonon energy			$26.34 \times 10^{-3}$				eV		
$D_{\text{op}}$	Cc	Coupling constant			$3.57 \times 10^{10}$				eV/m		
$i$	final	Final minima			$X[1, 2, 3, 4, 5, 6]$				—		

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*Table 428 Parameters of intervalley X to L optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
<b>Mechanism name: opl[1, 2, 3, 4, 5, 6, 7, 8]</b>									
<b>Description</b>									<b>Default</b>
$E_{op}$	E	Phonon energy	$23.24 \times 10^{-3}$						eV
$D_{op}$	Cc	Coupling constant	$6.63 \times 10^{10}$						eV/m
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]						—

*Table 429 Parameters of intervalley X to  $\Gamma$  optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X1	X2	X3	X4	X5	X6	Unit
<b>Mechanism name: opg</b>									
<b>Description</b>									<b>Default</b>
$E_{op}$	E	Phonon energy	$25.07 \times 10^{-3}$						eV
$D_{op}$	Cc	Coupling constant	$7.3 \times 10^{10}$						eV/m
$i$	final	Final minima	G						—

## L-Valley Scattering Mechanisms

The eight L-minima define the set of scattering mechanisms listed in [Table 430](#). By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL AlAs.conduction.C1.<valley>.<mechanism> ADD
```

```
MATERIAL AlAs.conduction.C1.<valley>.<mechanism> REMOVE
```

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Table 430 Scattering mechanisms for L-minima

Scattering mechanism	L1	L2	L3	L4	L5	L6	L7	L8
	Mechanism name							
Acoustic Phonon (elastic)	ac	ac	ac	ac	ac	ac	ac	ac
Polar Optical (intra)	pop	pop	pop	pop	pop	pop	pop	pop
Optical Phonon (intra)	opl	opl	opl	opl	opl	opl	opl	opl
Optical Phonon (inter)	opl2	opl1						
Optical Phonon (inter)	opl3	opl3	opl2	opl2	opl2	opl2	opl2	opl2
Optical Phonon (inter)	opl4	opl4	opl4	opl3	opl3	opl3	opl3	opl3
Optical Phonon (inter)	opl5	opl5	opl5	opl5	opl4	opl4	opl4	opl4
Optical Phonon (inter)	opl6	opl6	opl6	opl6	opl6	opl5	opl5	opl5
Optical Phonon (inter)	opl7	opl7	opl7	opl7	opl7	opl7	opl6	opl6
Optical Phonon (inter)	opl8	opl8	opl8	opl8	opl8	opl8	opl8	opl7
Optical Phonon (inter)	opx1	opx1	opx1	opx1	opx1	opx1	opx1	opx1
Optical Phonon (inter)	opx2	opx2	opx2	opx2	opx2	opx2	opx2	opx2
Optical Phonon (inter)	opx3	opx3	opx3	opx3	opx3	opx3	opx3	opx3
Optical Phonon (inter)	opx4	opx4	opx4	opx4	opx4	opx4	opx4	opx4
Optical Phonon (inter)	opx5	opx5	opx5	opx5	opx5	opx5	opx5	opx5
Optical Phonon (inter)	opx6	opx6	opx6	opx6	opx6	opx6	opx6	opx6
Optical Phonon (inter)	opg	opg	opg	opg	opg	opg	opg	opg
Ionized Impurity	II	II	II	II	II	II	II	II
Surface Roughness	SR	SR	SR	SR	SR	SR	SR	SR
Remote Coulomb	RC	RC	RC	RC	RC	RC	RC	RC

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each  $L$ -minimum, listed in [Table 430](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL AlAs.conduction.C1.<valley>.<mechanism>.<parameter> <value>
```

### Elastic Acoustic Phonon Scattering

[Table 431](#) lists the default parameter values of intravalley elastic *longitudinal* acoustic phonon scattering.

*Table 431 Parameters of elastic longitudinal acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	ac								
		Description	Default								
$\Delta_{ac}$	D	Acoustic deformation	7.0								eV
$v$	v	Velocity		4.4833×10 <sup>3</sup>							m/s
$i$	final	Final minima	L1	L2	L3	L4	L5	L6	L7	L8	—

### Polar-Optical Phonon Scattering

[Table 432](#) lists the default parameter values of intravalley polar-optical phonon scattering.

*Table 432 Parameters of polar-optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit
		Mechanism name:	pop								
		Description	Default								
$E_{op}$	E	Phonon energy		50.09×10 <sup>-3</sup>							eV
$i$	final	Final minima	L1	L2	L3	L4	L5	L6	L7	L8	—

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### Optical Phonon Scattering

Table 433 to Table 436 list the default parameter values of intravalley and intervalley optical phonon scattering.

Table 433 Parameters of intravalley optical phonon scattering

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit		
		Mechanism name:	opl										
		Description	Default										
$E_{op}$	E	Phonon energy	$26.97 \times 10^{-3}$										
$D_{op}$	Cc	Coupling constant	$8.02 \times 10^{10}$										
$i$	final	Final minima	L1	L2	L3	L4	L5	L6	L7	L8	—		

Table 434 Parameters of intervalley L to L optical phonon scattering

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit		
		Mechanism name:	opl[1, 2, 3, 4, 5, 6, 7, 8]										
		Description	Default										
$E_{op}$	E	Phonon energy	$26.97 \times 10^{-3}$										
$D_{op}$	Cc	Coupling constant	$8.02 \times 10^{10}$										
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]										

**Chapter 21: Aluminum Arsenide Material Model**  
 Conduction Band Model

*Table 435 Parameters of intervalley L to X optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit		
		<b>Mechanism name:</b>	<b>opx[1, 2, 3, 4, 5, 6]</b>										
		<b>Description</b>	<b>Default</b>										
$E_{\text{op}}$	E	Phonon energy	$23.24 \times 10^{-3}$										
$D_{\text{op}}$	CC	Coupling constant	$6.63 \times 10^{10}$										
$i$	final	Final minima	X[1, 2, 3, 4, 5, 6]										

*Table 436 Parameters of intervalley L to  $\Gamma$  optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L1	L2	L3	L4	L5	L6	L7	L8	Unit		
		<b>Mechanism name:</b>	<b>opg</b>										
		<b>Description</b>	<b>Default</b>										
$E_{\text{op}}$	E	Phonon energy	$25.07 \times 10^{-3}$										
$D_{\text{op}}$	CC	Coupling constant	$7.02 \times 10^{10}$										
$i$	final	Final minima	G										

## **$\Gamma$ -Valley Scattering Mechanisms**

The  $\Gamma$ -minimum defines the set of scattering mechanisms listed in [Table 437](#). By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL AlAs.conduction.C2.G.<mechanism> ADD
```

```
MATERIAL AlAs.conduction.C2.G.<mechanism> REMOVE
```

**Chapter 21: Aluminum Arsenide Material Model**

## Conduction Band Model

*Table 437 Scattering mechanisms for  $\Gamma$ -minimum*

Scattering mechanism	Mechanism name
Acoustic Phonon (elastic)	ac
Polar Optical (intra)	pop
Optical Phonon (inter)	opl1
Optical Phonon (inter)	opl2
Optical Phonon (inter)	opl3
Optical Phonon (inter)	opl4
Optical Phonon (inter)	opl5
Optical Phonon (inter)	opl6
Optical Phonon (inter)	opl7
Optical Phonon (inter)	opl8
Optical Phonon (inter)	opx1
Optical Phonon (inter)	opx2
Optical Phonon (inter)	opx3
Optical Phonon (inter)	opx4
Optical Phonon (inter)	opx5
Optical Phonon (inter)	opx6
Ionized Impurity	II
Surface Roughness	SR
Remote Coulomb	RC

## Parameters of Scattering Mechanisms

To change the default parameter values of the scattering mechanisms listed in [Table 437](#), use the following input file syntax:

```
MATERIAL AlAs.conduction.C2.G.<mechanism>.<parameter> <value>
```

### Elastic Acoustic Phonon Scattering

[Table 438](#) lists the default parameter values of intravalley elastic *longitudinal* acoustic phonon scattering.

*Table 438 Parameters of elastic longitudinal acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	ac	
		Description	Default	
$\Delta_{ac}$	D	Acoustic deformation	7.0	eV
$v$	v	Velocity	$4.4833 \times 10^3$	m/s
$i$	final	Final minima	G	—

### Polar-Optical Phonon Scattering

[Table 439](#) lists the default parameter values of intravalley polar-optical phonon scattering.

*Table 439 Parameters of polar-optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	pop	
		Description	Default	
$E_{op}$	E	Phonon energy	$50.09 \times 10^{-3}$	eV
$i$	final	Final minima	G	—

**Chapter 21: Aluminum Arsenide Material Model**  
 Conduction Band Model

### Optical Phonon Scattering

**Table 440** and **Table 441** list the default parameter values of intervalley optical phonon scattering.

*Table 440 Parameters of intervalley  $\Gamma$  to L optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
<b>Mechanism name:</b> opl[1, 2, 3, 4, 5, 6, 7, 8]				
<b>Description</b>				<b>Default</b>
$E_{\text{op}}$	E	Phonon energy	$25.07 \times 10^{-3}$	eV
$D_{\text{op}}$	Cc	Coupling constant	$7.02 \times 10^{10}$	eV/m
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]	—

*Table 441 Parameters of intervalley  $\Gamma$  to X optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
<b>Mechanism name:</b> opx[1, 2, 3, 4, 5, 6]				
<b>Description</b>				<b>Default</b>
$E_{\text{op}}$	E	Phonon energy	$25.07 \times 10^{-3}$	eV
$D_{\text{op}}$	Cc	Coupling constant	$7.3 \times 10^{10}$	eV/m
$i$	final	Final minima	X[1, 2, 3, 4, 5, 6]	—

---

## Ionized Impurity Scattering

Ionized impurity scattering is defined for each valley in a conduction band and is treated as an intravalley process by default, so that the final valley after scattering is the same as the initial valley.

*Table 442 Parameters of ionized impurity scattering*

Parameter symbol	Parameter name	Valley name:	All valleys	Unit
		Mechanism name:	II	
		Description	Default	
<i>i</i>	final	Final minimum	Same as initial minimum	–

## Ionized Impurity Empirical Rate Factor

The ionized impurity scattering model includes a scaling factor for the empirical correction of the calculated scattering rate as a function of doping density.

To redefine the default empirical factor, use the following input file syntax:

```
MATERIAL AlAs.conduction.IIfac N <Nvalue> [<Nvalue2>] <rule> <value>
```

Here, **IIfac** is a piecewise interpolation parameter that defines a correction factor **<value>** for a value **<Nvalue>** of the doping concentration **N**. The interpolation model used to return values between specified densities is given by **<rule>**, which might require an upper bound of the density [**<Nvalue2>**]. For a description of the interpolation parameter type, see [Interpolation Methods on page 301](#).

By default, the empirical correction for ionized impurity is 1.0. However, for electrons in AlAs, a non-unity default value is provided to best match experimental low-field concentration-dependent mobility.

## Surface Roughness Scattering

[Table 443](#) lists the default parameter values of surface roughness scattering. These parameters apply to all valleys and to all equivalent surface orientations.

*Table 443 Parameters of surface roughness scattering*

Parameter symbol	Parameter name	Mechanism name:	SR		Unit
		Description	Default		
$\Delta$	rms	RMS amplitude	0.33	0.65	nm
$L_c$	l	Correlation length	1.00	1.0	nm
$\langle hkl \rangle$	orient	Surface orientation	(001)	(110)	–
$i$	carrier	Carrier type	electrons	electrons	–

## Remote Coulomb Scattering

[Table 444](#) lists the default parameter values of remote Coulomb scattering, which is treated as an intravalley process. These parameters apply to all valleys.

*Table 444 Parameters of remote Coulomb scattering*

Parameter symbol	Parameter name	Mechanism name:	RC		Unit
		Description	Default		
$z_d$	zd	Depth of charge centroid	1.5		nm
$E_0$	E0	Minimum energy for tabulating rate	0		eV
$N_0$	N0	Minimum screening density	$5 \times 10^{15}$		$\text{cm}^{-3}$
$i$	final	Final minimum	Same as initial minimum		–

To define the interface charge density for remote Coulomb scattering, follow the descriptions in [Defining Interface Models on page 217](#). By default, no interface charge is applied.

## Valence Band Model

This section describes the valence band model.

### Band Edge Parameters

To change the default parameter values of the valence band container model, listed in [Table 445](#), use the following input file syntax:

```
MATERIAL AlAs.valence.<parameter> <value>
```

*Table 445 Parameters of valence band container model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Valence band energy with respect to vacuum	5.67	eV
$m_{dg_x}$	$dgx$	Hole density gradient effective x-mass	0.5	$m_e$
$m_{dg_y}$	$dgy$	Hole density gradient effective y-mass	0.5	$m_e$
$m_{dg_z}$	$dgz$	Hole density gradient effective z-mass	0.5	$m_e$
<b>k-p band structure model parameters</b>				
$L$	$L-kp$	Valence band parameter	0.0	$\hbar^2/2m$
$M$	$M-kp$	Valence band parameter	0.0	$\hbar^2/2m$
$N$	$N-kp$	Valence band parameter	0.0	$\hbar^2/2m$
$l$	$l-defpot$	Valence deformation potential	0.0	eV
$m$	$m-defpot$	Valence deformation potential	0.0	eV
$n$	$n-defpot$	Valence deformation potential	0.0	eV
$\Delta_{sso}$	$dsso$	Spin-orbit split energy	0.0	eV

## Chapter 21: Aluminum Arsenide Material Model

### Valence Band Model

To change the default parameter values of the valence bands in the container model, listed in [Table 446](#), use the following input file syntax:

```
MATERIAL AlAs.valence.<band>.<parameter> <value>
```

*Table 446 Parameters of valence band model*

Parameter symbol	Parameter name	Description	Default	Unit
<b>Heavy hole (HH) band</b>				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.0	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	6kp	—
<b>Light hole (LH) band</b>				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.0	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	6kp	—
<b>Spin split-off (SSO) band</b>				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.044	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	6kp	—

## Mobility Models

The valence band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models together with some phenomenological enhancement factors.

### Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 447](#), use the following input file syntax:

```
MATERIAL AlAs.valence.constant.<parameter> <value>
```

## Chapter 21: Aluminum Arsenide Material Model

### Valence Band Model

Table 447 Parameters of constant mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	150	$\text{cm}^2/\text{Vs}$
$\zeta$	zeta	Fitting parameter	2.1	—

## Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 448](#), use the following input file syntax:

```
MATERIAL AlAs.valence.Arora.<parameter> <value>
```

Table 448 Parameters of Arora mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min}$	mumin	Minimum mobility	54.3	$\text{cm}^2/\text{Vs}$
$\mu_{\max}$	mumax	Maximum mobility	150	$\text{cm}^2/\text{Vs}$
$N_0$	n0	Reference concentration	$2.35 \times 10^{17}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.88	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.33	—
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

## Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 449](#), use the following input file syntax:

```
MATERIAL AlAs.valence.Masetti.<parameter> <value>
```

## Chapter 21: Aluminum Arsenide Material Model

### Valence Band Model

*Table 449 Parameters of Masetti mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min 1}$	mumin1	Minimum mobility	75.0	cm <sup>2</sup> /Vs
$\mu_{\min 2}$	mumin2	Minimum mobility	75.0	cm <sup>2</sup> /Vs
$\mu_{\max}$	mumax	Maximum mobility	150	cm <sup>2</sup> /Vs
$\mu_1$	mul	Maximum mobility	1.0	cm <sup>2</sup> /Vs
$C_r$	cr	Reference concentration	$1.0 \times 10^{18}$	cm <sup>-3</sup>
$C_s$	cs	Reference solid solubility concentration	1.0	cm <sup>-3</sup>
$p_c$	pc	Fitting parameter	0.0	cm <sup>-3</sup>
$\alpha$	alpha	Fitting parameter	2.37	—
$\beta$	beta	Fitting parameter	2.0	—
$\zeta$	zeta	Fitting parameter	2.1	—

## Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 450](#), use the following input file syntax:

```
MATERIAL AlAs.valence.Yamaguchi.<parameter> <value>
```

*Table 450 Parameters of Yamaguchi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

## Perpendicular Field: Lombardi Mobility Model

To change the default parameter values of the Lombardi mobility model, listed in [Table 451](#), use the following input file syntax:

```
MATERIAL AlAs.valence.Lombardi.<parameter> <value>
```

*Table 451 Parameters of Lombardi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
A	a	Fitting parameter	2.0	—
B	b	Fitting parameter	$9.925 \times 10^6$	cm/s
C	c	Fitting parameter	$2.947 \times 10^3$	$\text{cm}^{5/3} \text{V}^{-2/3} \text{s}^{-1}$
$\alpha$	alpha	Fitting parameter	0.0	$\text{cm}^3$
$\delta$	delta	Fitting parameter	$2.0546 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$2.0546 \times 10^{30}$	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	1.0	—
$\lambda$	lambda	Fitting parameter	0.0317	—
v	nu	Fitting parameter	1.0	—
$N_0$	n0	Fitting parameter	1.0	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	1.0	$\text{cm}^{-3}$
$l_{\text{crit}}$	lcrit	Critical length	$1 \times 10^{-6}$	cm

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in [Table 452](#), use the following input file syntax:

```
MATERIAL AlAs.valence.Caughey.<parameter> <value>
```

## Chapter 21: Aluminum Arsenide Material Model

### Valence Band Model

Table 452 Parameters of Caughey–Thomas mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$4.5 \times 10^6$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	0.52	—
$\beta_0$	beta0	Fitting parameter	1.213	—
$\beta_{\text{exp}}$	bexp	Fitting parameter	0.17	—
$\alpha$	alpha	Fitting parameter	0.0	—

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 453](#). To change the default mobility model, use the following input file syntax:

```
MATERIAL AlAs.valence.mobility.<model> <value>
```

Table 453 Parameters of default mobility model

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley valence band model consists of the valley minima listed in [Table 454](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL AlAs.valence.<band>.<valley> REMOVE
```

### Note:

The valence band analytic valley approximation is used only as a way to define density-of-states for drift-diffusion simulations and to define the valley minima in response to stress.

## Chapter 21: Aluminum Arsenide Material Model

### Valence Band Model

*Table 454 Names of valence band minima*

Valence band minima	Band name	Valley name
Heavy hole	HH	vhh
Light hole	LH	vlh
Spin split-off	SSO	vsso

## Position and Orientation

The position and orientation of the HH, LH, and SSO valley minima are identical. [Table 455](#) shows the default values. To change the default values, use the following input file syntax:

```
MATERIAL AlAs.valence.<band>.<valley>.min.<parameter> <value>
```

*Table 455 Position and orientation parameters of HH, LH, and SSO valley minima*

Parameter symbol	Parameter name	Description	Default	Unit
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.0	$2\pi/a$
x	x	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
y	y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
z	z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$

## Parameters

To change the valley minima model parameters, listed in [Table 456](#), for each valley listed in [Table 454](#), use the following input file syntax:

```
MATERIAL AlAs.valence.<band>.<valley>.parameters <value>
```

*Table 456 Parameters of valence band minima*

Parameter symbol	Parameter name	Description	Default	Unit
<b>Heavy hole (HH) band</b>				
E	E	Minima with respect to band edge	0.0	eV

## Chapter 21: Aluminum Arsenide Material Model

### Valence Band Model

Table 456 Parameters of valence band minima (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$m_x$	mx	Longitudinal effective mass	0.76	$m_e$
$m_y$	my	Transverse effective mass	0.76	$m_e$
$m_z$	mz	Transverse effective mass	0.76	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	0.0	eV
<b>Light hole (LH) band</b>				
$E$	E	Minima with respect to band edge	0.0	eV
$m_x$	mx	Longitudinal effective mass	0.15	$m_e$
$m_y$	my	Transverse effective mass	0.15	$m_e$
$m_z$	mz	Transverse effective mass	0.15	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	0.0	eV
<b>Spin split-off (SSO) band</b>				
$E$	E	Minima with respect to band edge	0.3	eV
$m_x$	mx	Longitudinal effective mass	0.28	$m_e$
$m_y$	my	Transverse effective mass	0.28	$m_e$
$m_z$	mz	Transverse effective mass	0.28	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	0.0	eV

## **Heavy-Hole Band Scattering Mechanisms**

There are no heavy-hole band scattering mechanisms defined in the current version of Garand.

---

## **Light-Hole Band Scattering Mechanisms**

There are no light-hole band scattering mechanisms defined in the current version of Garand.

---

## **Spin Split-Off Band Scattering Mechanisms**

There are no spin split-off band scattering mechanisms defined in the current version of Garand.

## Silicon Germanium Binary Alloy Material Model

---

*This chapter describes the  $\text{Si}_{1-x}\text{Ge}_x$  binary alloy material model.*

---

### Bulk Material Model

This section describes the bulk material model for the  $\text{Si}_{1-x}\text{Ge}_x$  binary alloy material.

---

#### Parameters of Bulk Material Model

To change the default parameter values in [Table 457](#), use the following input file syntax:

```
MATERIAL SiliconGermanium.<parameter> <value>
```

*Table 457 Bulk material model parameters*

Parameter symbol	Parameter name	Description	Default	Unit
<b>Binary material-specific properties</b>				
$x$	x_fraction	Binary alloy fraction	0.0	—
<b>Crystal lattice and orientation in simulation domain</b>				

**Chapter 22: Silicon Germanium Binary Alloy Material Model**  
**Bulk Material Model**

*Table 457 Bulk material model parameters (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$ a $	a	Magnitude of lattice vector $a$	$x = 0.0 \quad 5.43060$ $x = 0.1 \quad 5.45090$ $x = 0.2 \quad 5.47175$ $x = 0.3 \quad 5.49313$ $x = 0.4 \quad 5.51506$ $x = 0.5 \quad 5.53753$ $x = 0.6 \quad 5.56054$ $x = 0.7 \quad 5.58409$ $x = 0.8 \quad 5.60819$ $x = 0.9 \quad 5.63282$ $x = 1.0 \quad 5.65800$	Å
$ b $	b	Magnitude of lattice vector $b$	$x = 0.0 \quad 5.43060$ $x = 0.1 \quad 5.45090$ $x = 0.2 \quad 5.47175$ $x = 0.3 \quad 5.49313$ $x = 0.4 \quad 5.51506$ $x = 0.5 \quad 5.53753$ $x = 0.6 \quad 5.56054$ $x = 0.7 \quad 5.58409$ $x = 0.8 \quad 5.60819$ $x = 0.9 \quad 5.63282$ $x = 1.0 \quad 5.65800$	Å
$ c $	c	Magnitude of lattice vector $c$	$x = 0.0 \quad 5.43060$ $x = 0.1 \quad 5.45090$ $x = 0.2 \quad 5.47175$ $x = 0.3 \quad 5.49313$ $x = 0.4 \quad 5.51506$ $x = 0.5 \quad 5.53753$ $x = 0.6 \quad 5.56054$ $x = 0.7 \quad 5.58409$ $x = 0.8 \quad 5.60819$ $x = 0.9 \quad 5.63282$ $x = 1.0 \quad 5.65800$	Å

**Chapter 22: Silicon Germanium Binary Alloy Material Model**  
**Bulk Material Model**

*Table 457 Bulk material model parameters (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$\alpha$	alpha	Angle between $b$ and $c$	90	degree
$\beta$	beta	Angle between $c$ and $a$	90	degree
$\gamma$	gamma	Angle between $a$ and $b$	90	degree
$\langle hkl \rangle_x$	x	Orientation in the x-direction	1 1 0	—
$\langle hkl \rangle_z$	z	Orientation in the z-direction	0 0 1	—
<b>Bulk electrical and mechanical properties</b>				
$\kappa$	permittivity	Relative dielectric constant	$\begin{cases} x = 0.0 & 11.7 \\ x = 1.0 & 16.2 \end{cases}$	—
$\kappa_\infty$	k_inf	High-frequency permittivity	$\begin{cases} x = 0.0 & 11.7 \\ x = 1.0 & 16.2 \end{cases}$	—
$\rho$	density	Mass density	$\begin{cases} x = 0.0 & 2.329 \\ x = 1.0 & 5.32 \end{cases}$	g/cm <sup>3</sup>
$C_{11}$	c11	Elastic stiffness matrix element	$\begin{cases} x = 0.0 & 168.3 \\ x = 1.0 & 132.8 \end{cases}$	GPa
$C_{12}$	c12	Elastic stiffness matrix element	$\begin{cases} x = 0.0 & 66.8 \\ x = 1.0 & 46.8 \end{cases}$	GPa
$C_{44}$	c44	Elastic stiffness matrix element	$\begin{cases} x = 0.0 & 79.9 \\ x = 1.0 & 66.57 \end{cases}$	GPa

## Band-to-Band Tunneling Parameters

To change the default parameter values for the Kane model, listed in [Table 458](#), use the following input file syntax:

```
MATERIAL SiliconGermanium.BTBT.<parameter> <value>
```

*Table 458 Band-to-band tunneling parameters*

Parameter symbol	Parameter name	Description	Default	Unit
$D_{TA}$	DTA	Acoustic phonon deformation potential	$\left\{ \begin{array}{ll} x = 0.1 & 2.29 \times 10^{10} \\ x = 0.2 & 2.12 \times 10^{10} \\ x = 0.3 & 1.96 \times 10^{10} \\ x = 0.4 & 1.79 \times 10^{10} \\ x = 0.5 & 1.63 \times 10^{10} \\ x = 0.6 & 1.46 \times 10^{10} \\ x = 0.7 & 1.30 \times 10^{10} \\ x = 0.8 & 1.13 \times 10^{10} \\ x = 0.9 & 0.97 \times 10^{10} \end{array} \right.$	eV
$\epsilon_{TA}$	epsilonTA	Acoustic phonon energy	$\left\{ \begin{array}{ll} x = 0.1 & 17.96 \times 10^3 \\ x = 0.2 & 16.92 \times 10^3 \\ x = 0.3 & 15.88 \times 10^3 \\ x = 0.4 & 14.84 \times 10^3 \\ x = 0.5 & 13.80 \times 10^3 \\ x = 0.6 & 12.76 \times 10^3 \\ x = 0.7 & 11.72 \times 10^3 \\ x = 0.8 & 10.68 \times 10^3 \\ x = 0.9 & 9.64 \times 10^3 \end{array} \right.$	eV

## Chapter 22: Silicon Germanium Binary Alloy Material Model

### Conduction Band Model

---

## Conduction Band Model

This section describes the conduction band model.

---

### Band Edge Parameters

To change the default parameter values of the conduction band container model, listed in [Table 459](#), use the following input file syntax:

```
MATERIAL SiliconGermanium.conduction.<parameter> <value>
```

*Table 459 Parameters of conduction band container model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Conduction band energy with respect to vacuum	$\begin{cases} x = 0.0 & 4.0727 \\ x = 0.1 & 4.0290 \\ x = 0.2 & 4.0210 \\ x = 0.3 & 3.9980 \\ x = 0.4 & 3.9890 \\ x = 0.5 & 3.9840 \\ x = 0.6 & 3.9380 \\ x = 0.7 & 3.8870 \\ x = 0.8 & 3.8320 \\ x = 0.9 & 3.8360 \\ x = 1.0 & 4.0000 \end{cases}$	eV
$m_{dg_x}$	$dgx$	Electron density gradient effective x-mass	0.3	$m_e$
$m_{dg_y}$	$dgy$	Electron density gradient effective y-mass	0.3	$m_e$
$m_{dg_z}$	$dgz$	Electron density gradient effective z-mass	0.3	$m_e$

To change the default parameter values of the conduction bands in the container model, listed in [Table 460](#) and [Table 461](#), use the following input file syntax:

```
MATERIAL AlAs.conduction.<band>.<parameter> <value>
```

## Chapter 22: Silicon Germanium Binary Alloy Material Model

### Conduction Band Model

*Table 460 Parameters of conduction band C1*

Parameter symbol	Parameter name	Description	Default	Unit
<i>E</i>	<i>E</i>	Conduction band energy with respect to vacuum	0.0	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	ema	—

*Table 461 Parameters of conduction band C2*

Parameter symbol	Parameter name	Description	Default	Unit
<i>E</i>	<i>E</i>	Conduction band energy with respect to vacuum	$\begin{cases} x = 0.0 & 2.8954 \\ x = 0.1 & 2.611482 \\ x = 0.2 & 2.317326 \\ x = 0.3 & 2.027092 \\ x = 0.4 & 1.74078 \\ x = 0.5 & 1.43339 \\ x = 0.6 & 1.134922 \\ x = 0.7 & 0.835376 \\ x = 0.8 & 0.534752 \\ x = 0.9 & 0.29805 \\ x = 1.0 & 0.15147 \end{cases}$	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	ema	—

## Mobility Models

The conduction band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models.

### Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 462](#), use the following input file syntax:

```
MATERIAL SiliconGermanium.conduction.constant.<parameter> <value>
```

**Chapter 22: Silicon Germanium Binary Alloy Material Model**  
 Conduction Band Model

*Table 462 Parameters of constant mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	$\begin{cases} x = 0.1 & 976 \\ x = 0.2 & 568.7 \\ x = 0.3 & 290.9 \\ x = 0.4 & 250.0 \\ x = 0.5 & 276.7 \\ x = 0.6 & 373.1 \\ x = 0.7 & 378.3 \\ x = 0.8 & 392.8 \\ x = 0.9 & 1037.7 \end{cases}$	cm <sup>2</sup> /Vs
$\zeta$	zeta	Fitting parameter	$\begin{cases} x = 0.1 & 2.4 \\ x = 0.2 & 2.3 \\ x = 0.3 & 2.2 \\ x = 0.4 & 2.1 \\ x = 0.5 & 2.0 \\ x = 0.6 & 1.9 \\ x = 0.7 & 1.8 \\ x = 0.8 & 1.7 \\ x = 0.9 & 1.6 \end{cases}$	—

## Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 463](#), use the following input file syntax:

```
MATERIAL SiliconGermanium.conduction.Arora.<parameter> <value>
```

**Chapter 22: Silicon Germanium Binary Alloy Material Model**  
 Conduction Band Model

*Table 463 Parameters of Arora mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\max}$	mumax	Maximum mobility	$\begin{cases} x = 0.1 & 976 \\ x = 0.2 & 568.7 \\ x = 0.3 & 290.9 \\ x = 0.4 & 250.0 \\ x = 0.5 & 276.7 \\ x = 0.6 & 373.1 \\ x = 0.7 & 378.3 \\ x = 0.8 & 392.8 \\ x = 0.9 & 1037.7 \end{cases}$	$\text{cm}^2/\text{Vs}$
$\mu_{\min}$	mumin	Minimum mobility	88.0	$\text{cm}^2/\text{Vs}$
$N_0$	n0	Reference concentration	$1.25 \times 10^{17}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.88	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.33	—
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

### Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 464](#), use the following input file syntax:

```
MATERIAL SiliconGermanium.conduction.Masetti.<parameter> <value>
```

**Chapter 22: Silicon Germanium Binary Alloy Material Model**  
 Conduction Band Model

*Table 464 Parameters of Masetti mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\max}$	mumax	Maximum mobility	$\begin{cases} x = 0.1 & 976 \\ x = 0.2 & 568.7 \\ x = 0.3 & 290.9 \\ x = 0.4 & 250.0 \\ x = 0.5 & 276.7 \\ x = 0.6 & 373.1 \\ x = 0.7 & 378.3 \\ x = 0.8 & 392.8 \\ x = 0.9 & 1037.7 \end{cases}$	$\text{cm}^2/\text{Vs}$
$\mu_{\min1}$	mumin1	Minimum mobility	52.2	$\text{cm}^2/\text{Vs}$
$\mu_{\min2}$	mumin2	Minimum mobility	52.2	$\text{cm}^2/\text{Vs}$
$\mu_1$	mul	Maximum mobility	43.4	$\text{cm}^2/\text{Vs}$
$C_r$	cr	Reference concentration	$9.68 \times 10^{16}$	$\text{cm}^{-3}$
$C_s$	cs	Reference solid solubility concentration	$3.43 \times 10^{20}$	$\text{cm}^{-3}$
$p_c$	pc	Fitting parameter	0.0	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.68	—
$\beta$	beta	Fitting parameter	2.0	—
$\zeta$	zeta	Fitting parameter	$\begin{cases} x = 0.1 & 2.4 \\ x = 0.2 & 2.3 \\ x = 0.3 & 2.2 \\ x = 0.4 & 2.1 \\ x = 0.5 & 2.0 \\ x = 0.6 & 1.9 \\ x = 0.7 & 1.8 \\ x = 0.8 & 1.7 \\ x = 0.9 & 1.6 \end{cases}$	—

## Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 465](#), use the following input file syntax:

```
MATERIAL SiliconGermanium.conduction.Yamaguchi.<parameter> <value>
```

*Table 465 Parameters of Yamaguchi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

## Perpendicular Field: Lombardi Mobility Model

To change the default parameter values of the Lombardi mobility model, listed in [Table 466](#), use the following input file syntax:

```
MATERIAL SiliconGermanium.conduction.Lombardi.<parameter> <value>
```

*Table 466 Parameters of Lombardi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$A$	a	Fitting parameter	2.0	—
$B$	b	Fitting parameter	$4.75 \times 10^7$	cm/s
$C$	c	Fitting parameter	$5.80 \times 10^2$	$\text{cm}^{5/3} \text{V}^{-2/3} \text{s}^{-1}$
$\alpha$	alpha	Fitting parameter	0.0	$\text{cm}^3$
$\delta$	delta	Fitting parameter	$5.82 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$5.82 \times 10^{30}$	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	1.0	—
$\lambda$	lambda	Fitting parameter	0.125	—
$\nu$	nu	Fitting parameter	1.0	—

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 Conduction Band Model

*Table 466 Parameters of Lombardi mobility model (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$N_0$	n0	Fitting parameter	1.0	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	1.0	$\text{cm}^{-3}$
$l_{\text{crit}}$	lcrit	Critical length	$1 \times 10^{-6}$	cm

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in [Table 467](#), use the following input file syntax:

```
MATERIAL SiliconGermanium.conduction.Caughey.<parameter> <value>
```

*Table 467 Parameters of Caughey–Thomas mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$1.07 \times 10^7$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	0.87	–
$\beta_0$	beta0	Fitting parameter	1.109	–
$\beta_{\text{exp}}$	bexp	Fitting parameter	0.66	–
$\alpha$	alpha	Fitting parameter	0.0	–

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 468](#). To change the default mobility model, use the following input file syntax:

```
MATERIAL SiliconGermanium.conduction.mobility.<model> <value>
```

## Chapter 22: Silicon Germanium Binary Alloy Material Model

### Conduction Band Model

Table 468 Parameters of default mobility model

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley conduction band model consists of the valley minima listed in [Table 469](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL SiliconGermanium.conduction.<band>.<valley> REMOVE
```

Table 469 Names of conduction band minima

Conduction band minima	Valley name
C1	
X	X1, X2, X3, X4, X5, X6
L	L1, L2, L3, L4, L5, L6, L7, L8
C2	
$\Gamma$	G

## Position and Orientation

Valley minima differ in their position and orientation, the default values of which are shown in [Table 470](#), [Table 471](#), and [Table 472](#).

To change default values, use the following input file syntax:

```
MATERIAL SiliconGermanium.conduction.C1.<valley>.min.<parameter> <value>
```

**Chapter 22: Silicon Germanium Binary Alloy Material Model**  
 Conduction Band Model

*Table 470 Position and orientation parameters of L-minima of conduction band*

Parameter symbol	Parameter name	Description	Default	Unit
<b>L1</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 1 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L2</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 1 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	1 -1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 1 0	$\langle hkl \rangle$
<b>L3</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 -0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	-1 -1 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 -1 -2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L4</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 -0.5 0.5	$2\pi/a$
x	X	Orientation of the x-axis	1 -1 1	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	-1 1 2	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$

**Chapter 22: Silicon Germanium Binary Alloy Material Model**  
 Conduction Band Model

*Table 470 Position and orientation parameters of L-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
<b>L5</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 0.5 -0.5	$2\pi/a$
$x$	X	Orientation of the x-axis	1 1 -1	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	1 1 2	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L6</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 0.5 -0.5	$2\pi/a$
$x$	X	Orientation of the x-axis	-1 1 -1	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	1 -1 -2	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	1 -1 0	$\langle hkl \rangle$
<b>L7</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 -0.5 -0.5	$2\pi/a$
$x$	X	Orientation of the x-axis	-1 -1 -1	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 -1 2	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	-1 1 0	$\langle hkl \rangle$
<b>L8</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 -0.5 -0.5	$2\pi/a$
$x$	X	Orientation of the x-axis	1 -1 -1	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	1 -1 2	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	-1 -1 0	$\langle hkl \rangle$

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 Conduction Band Model

*Table 471 Position and orientation parameters of  $\Gamma$ -minimum of conduction band*

Parameter symbol	Parameter name	Description	Default	Unit
G				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$

*Table 472 Position and orientation parameters of X-minima of conduction band*

Parameter symbol	Parameter name	Description	Default	Unit
X1				
$k_0$	pos	Position within the Brillouin zone	0.85 0.0 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
X2				
$k_0$	pos	Position within the Brillouin zone	-0.85 0.0 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
X3				
$k_0$	pos	Position within the Brillouin zone	0.0 0.85 0.0	$2\pi/a$

**Chapter 22: Silicon Germanium Binary Alloy Material Model**  
 Conduction Band Model

*Table 472 Position and orientation parameters of X-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$x$	X	Orientation of the x-axis	0 1 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X4</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 -0.85 0.0	$2\pi/a$
$x$	X	Orientation of the x-axis	0 1 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$
<b>X5</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.85	$2\pi/a$
$x$	X	Orientation of the x-axis	0 0 1	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 -1 0	$\langle hkl \rangle$
<b>X6</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 -0.85	$2\pi/a$
$x$	X	Orientation of the x-axis	0 1 0	$\langle hkl \rangle$
$y$	Y	Orientation of the y-axis	-1 0 0	$\langle hkl \rangle$
$z$	Z	Orientation of the z-axis	0 -1 0	$\langle hkl \rangle$

## Parameters

To change the default parameter values of the valley minima models, listed in the following tables, for each valley listed in [Table 473](#), use the following input file syntax:

```
MATERIAL SiliconGermanium.conduction.C1.<valley>.<parameter> <value>
```

**Note:**

By default, all  $X$ -minima have the same parameter values, and all  $L$ -minima have the same parameter values.

*Table 473 Parameters of L-valley model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	<code>E</code>	Minima energy with respect to band edge	$\begin{cases} x = 0.0 & 0.96534 \\ x = 0.1 & 0.87066 \\ x = 0.2 & 0.763178 \\ x = 0.3 & 0.657055 \\ x = 0.4 & 0.55229 \\ x = 0.5 & 0.423883 \\ x = 0.6 & 0.301834 \\ x = 0.7 & 0.176143 \\ x = 0.8 & 0.04681 \\ x = 0.85 & 0.0 \\ x = 0.9 & 0.0 \\ x = 1.0 & 0.0 \end{cases}$	eV
$m_x$	<code>mx</code>	Longitudinal effective mass	$\begin{cases} x < 0.9 & 1.643 \\ x \geq 0.9 & 1.588 \end{cases}$	$m_e$
$m_y$	<code>my</code>	Transverse effective mass	$\begin{cases} x < 0.9 & 0.126 \\ x \geq 0.9 & 0.082 \end{cases}$	$m_e$
$m_z$	<code>mz</code>	Transverse effective mass	$\begin{cases} x < 0.9 & 0.126 \\ x \geq 0.9 & 0.082 \end{cases}$	$m_e$
$\alpha$	<code>a</code>	Valley nonparabolicity factor	$\begin{cases} x < 0.9 & 0.3 \\ x \geq 0.9 & 0.33 \end{cases}$	—
$\Xi_u$	<code>xi_u</code>	Uniaxial deformation potential	$\begin{cases} x = 0.0 & 11.5 \\ x = 1.0 & 16.7 \end{cases}$	eV

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 Conduction Band Model

*Table 473 Parameters of L-valley model (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$\Xi_d$	xi_d	Dilatation deformation potential	-6.58	eV
$\Xi'_u$	xi_u_prime	Uniaxial mass deformation	0.0	eV
$M$	M	Fitting parameter for electron mass	0.0	—
$\Delta$	delta	Fitting parameter for electron mass	0.0	eV

*Table 474 Parameters of X-valley model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Minima energy with respect to band edge	$\begin{cases} x \leq 0.85 & 0.0 \\ x = 0.9 & 0.050042 \\ x = 1.0 & 0.19953 \end{cases}$	eV
$m_x$	mx	Longitudinal effective mass	$\begin{cases} x < 0.9 & 0.9163 \\ x \geq 0.9 & 1.3530 \end{cases}$	$m_e$
$m_y$	my	Transverse effective mass	$\begin{cases} x < 0.9 & 0.198207 \\ x \geq 0.9 & 0.288000 \end{cases}$	$m_e$
$m_z$	mz	Transverse effective mass	$\begin{cases} x < 0.9 & 0.198207 \\ x \geq 0.9 & 0.288000 \end{cases}$	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.5	—
$\Xi_u$	xi_u	Uniaxial deformation potential	$\begin{cases} x = 0.0 & 9.16 \\ x = 1.0 & 9.42 \end{cases}$	eV

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 Conduction Band Model

*Table 474 Parameters of X-valley model (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$\Xi_d$	xi_d	Dilatation deformation potential	$\begin{cases} x = 0.0 & 0.77 \\ x = 1.0 & -0.59 \end{cases}$	eV
$\Xi'_u$	xi_u_prime	Uniaxial mass deformation	$\begin{cases} x = 0.0 & 7.00 \\ x = 1.0 & 8.07 \end{cases}$	eV
$M$	M	Fitting parameter for electron mass	$\begin{cases} x = 0.0 & 1.20 \\ x = 1.0 & 1.00 \end{cases}$	—
$\Delta$	delta	Fitting parameter for electron mass	$\begin{cases} x = 0.0 & 0.53 \\ x = 1.0 & 0.90 \end{cases}$	eV

*Table 475 Parameters of  $\Gamma$ -valley model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Minima energy with respect to band edge	0.0	eV
$m_x$	mx	Longitudinal effective mass	$\begin{cases} x < 0.9 & 1.987 \\ x \geq 0.9 & 0.037 \end{cases}$	$m_e$
$m_y$	my	Transverse effective mass	$\begin{cases} x < 0.9 & 0.229 \\ x \geq 0.9 & 0.037 \end{cases}$	$m_e$
$m_z$	mz	Transverse effective mass	$\begin{cases} x < 0.9 & 0.229 \\ x \geq 0.9 & 0.037 \end{cases}$	$m_e$
$\alpha$	a	Valley nonparabolicity factor	$\begin{cases} x < 0.9 & 0.0 \\ x \geq 0.9 & 0.85 \end{cases}$	—

## Chapter 22: Silicon Germanium Binary Alloy Material Model

### Conduction Band Model

Table 475 Parameters of  $\Gamma$ -valley model (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$\Xi_u$	xi_u	Uniaxial deformation potential	$\begin{cases} x = 0.0 & 9.16 \\ x = 1.0 & 9.42 \end{cases}$	eV
$\Xi_d$	xi_d	Dilatation deformation potential	$\begin{cases} x = 0.0 & 0.77 \\ x = 1.0 & -0.59 \end{cases}$	eV
$\Xi'_u$	xi_u_prime	Uniaxial mass deformation	$\begin{cases} x = 0.0 & 7.00 \\ x = 1.0 & 8.07 \end{cases}$	eV
$M$	M	Fitting parameter for electron mass	0.0	—
$\Delta$	delta	Fitting parameter for electron mass	0.0	eV

## L-Valley Scattering Mechanisms

The eight  $L$ -minima define a set of scattering mechanisms that is consistent with both the silicon and germanium definitions. By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL SiliconGermanium.conduction.C1.<valley>.<mechanism> ADD
MATERIAL SiliconGermanium.conduction.C1.<valley>.<mechanism> REMOVE
```

## Parameters

By default, the equivalent scattering mechanisms defined for each  $L$ -minimum have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL SiliconGermanium.conduction.C1.<valley>.<mechanism>.<parameter>
<value>
```

### Inelastic Acoustic Phonon Scattering

Both silicon and germanium phonon modes are included for SiGe. In each case, the squared deformation potential is weighted by the mole fraction,  $x$  (germanium modes) or  $1-x$  (silicon modes).

The default parameter values of intravalley acoustic phonon scattering are consistent with the values used for silicon (see [Table 99 on page 408](#) and [Table 100 on page 408](#)) and germanium (see [Table 162 on page 455](#) and [Table 163 on page 456](#)).

### Optical Phonon Scattering

Both silicon and germanium phonon modes are included for SiGe. In each case, the squared coupling constant is weighted by the mole fraction,  $x$  (germanium modes) or  $1-x$  (silicon modes).

The default parameter values of optical phonon scattering are consistent with the values used for silicon (see [Table 101 on page 409](#) to [Table 103 on page 410](#)) and germanium (see [Table 164 on page 457](#) to [Table 168 on page 458](#)).

### Alloy Potential Scattering

[Table 476](#) lists the default parameter values of intravalley alloy potential scattering.

*Table 476 Parameters of alloy potential scattering*

Parameter symbol	Parameter name	Valley name:	L[1, 2, 3, 4, 5, 6, 7, 8]	Unit
		Mechanism name:	al	
		Description	Default	
$U$	$U$	Alloy potential	1.0	eV
$i$	final	Final minima	L[1, 2, 3, 4, 5, 6, 7, 8]	—

### $\Gamma$ -Valley Scattering Mechanisms

The  $\Gamma$ -minimum defines a set of scattering mechanisms that is consistent with both the silicon and germanium definitions. By default, all these scattering mechanisms are added to the default scattering model.

## Chapter 22: Silicon Germanium Binary Alloy Material Model

### Conduction Band Model

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL SiliconGermanium.conduction.C2.G.<mechanism> ADD
```

```
MATERIAL SiliconGermanium.conduction.C2.G.<mechanism> REMOVE
```

## Parameters of Scattering Mechanisms

To change the parameter values for the  $\Gamma$ -minimum, use the following input file syntax:

```
MATERIAL SiliconGermanium.conduction.C2.G.<mechanism>. <parameter> <value>
```

### Inelastic Acoustic Phonon Scattering

Both silicon and germanium phonon modes are included for SiGe. In each case, the squared deformation potential is weighted by the mole fraction,  $x$  (germanium modes) or  $1-x$  (silicon modes).

The default parameter values of intravalley acoustic phonon scattering are consistent with the values used for silicon (see [Table 105 on page 412](#) and [Table 106 on page 412](#)) and germanium (see [Table 170 on page 460](#) and [Table 171 on page 461](#)).

### Optical Phonon Scattering

Both silicon and germanium phonon modes are included for SiGe. In each case, the squared coupling constant is weighted by the mole fraction,  $x$  (germanium modes) or  $1-x$  (silicon modes).

The default parameter values of optical phonon scattering are consistent with the values used for silicon (see [Table 107 on page 413](#) and [Table 108 on page 413](#)) and germanium (see [Table 172 on page 461](#) and [Table 173 on page 462](#)).

### Alloy Potential Scattering

[Table 477](#) lists the default parameter values of intravalley alloy potential scattering.

*Table 477 Parameters of alloy potential scattering*

Parameter symbol	Parameter name	Valley name: G	Unit	
		Mechanism name: al		
		Description	Default	
$U$	$U$	Alloy potential	1.0	eV
$i$	final	Final minima	G	—

## X-Valley Scattering Mechanisms

The six *X*-minima define a set of scattering mechanisms that is consistent with both the silicon and germanium definitions. By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL SiliconGermanium.conduction.C1.<valley>.<mechanism> ADD
```

```
MATERIAL SiliconGermanium.conduction.C1.<valley>.<mechanism> REMOVE
```

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each *X*-minima have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL SiliconGermanium.conduction.C1.<valley>.<mechanism>.<parameter> <value>
```

### Inelastic Acoustic Phonon Scattering

Both silicon and germanium phonon modes are included for SiGe. In each case, the squared deformation potential is weighted by the mole fraction,  $x$  (germanium modes) or  $1-x$  (silicon modes).

The default parameter values of intravalley acoustic phonon scattering are consistent with the values used for silicon (see [Table 88 on page 402](#) and [Table 89 on page 402](#)) and germanium (see [Table 155 on page 451](#) and [Table 156 on page 451](#)).

### Optical Phonon Scattering

Both silicon and germanium phonon modes are included for SiGe. In each case, the squared coupling constant is weighted by the mole fraction,  $x$  (germanium modes) or  $1-x$  (silicon modes).

The default parameter values of optical phonon scattering are consistent with the values used for silicon (see [Table 90 on page 403](#) to [Table 95 on page 405](#)) and germanium (see [Table 157 on page 452](#) to [Table 160 on page 453](#)).

### Alloy Potential Scattering

Table 478 lists the default parameter values of intravalley alloy potential scattering.

Table 478 Parameters of alloy potential scattering

Parameter symbol	Parameter name	Valley name:	X[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	al	
		Description	Default	
$U$	$U$	Alloy potential	1.0	eV
$i$	final	Final minima	X[1, 2, 3, 4, 5, 6]	—

---

### Surface Roughness Scattering

Table 479 lists the default parameter values of surface roughness scattering. These parameters apply to all valleys and to all equivalent surface orientations.

Table 479 Parameters of surface roughness scattering

Parameter symbol	Parameter name	Mechanism name:	SR	Unit	
		Description	Default		
$\Delta$	rms	RMS amplitude	0.33	0.65	nm
$L_c$	l	Correlation length	1.00	1.00	nm
$\langle hkl \rangle$	orient	Surface orientation	(001)	(110)	—
$i$	carrier	Carrier type	electrons	electrons	—

---

## Remote Coulomb Scattering

[Table 480](#) lists the default parameter values of remote Coulomb scattering, which is treated as an intravalley process. These parameters apply to all valleys.

*Table 480 Parameters of remote Coulomb scattering*

Parameter symbol	Parameter name	Mechanism name:	RC	Unit
		Description		
$z_d$	zd	Depth of charge centroid	1.5	nm
$E_0$	e0	Minimum energy for tabulating rate	0	eV
$N_0$	n0	Minimum screening density	$5 \times 10^{15}$	cm <sup>-3</sup>
$i$	final	Final minimum	Same as initial minimum	–

To define the interface charge density for remote Coulomb scattering, follow the descriptions in [Defining Interface Models on page 217](#). By default, no interface charge is applied.

---

## Valence Band Model

This section describes the valence band model.

---

## Band Edge Parameters

To change the default parameter values of the valence band container model, listed in [Table 481](#), use the following input file syntax:

```
MATERIAL SiliconGermanium.valence.<parameter> <value>
```

**Chapter 22: Silicon Germanium Binary Alloy Material Model**  
**Valence Band Model**

*Table 481 Parameters of valence band container model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Valence band energy with respect to vacuum	$\begin{cases} x = 0.0 & 5.19686 \\ x = 0.1 & 5.099 \\ x = 0.2 & 5.051 \\ x = 0.3 & 4.988 \\ x = 0.4 & 4.939 \\ x = 0.5 & 4.919 \\ x = 0.6 & 4.853 \\ x = 0.7 & 4.787 \\ x = 0.8 & 4.722 \\ x = 0.9 & 4.656 \\ x = 1.0 & 4.6638 \end{cases}$	eV
$m_{dg_x}$	$dgx$	Hole density gradient effective x-mass	0.5	$m_e$
$m_{dg_y}$	$dgy$	Hole density gradient effective y-mass	0.5	$m_e$
$m_{dg_z}$	$dgz$	Hole density gradient effective z-mass	0.5	$m_e$
<b>k-p band structure model parameters</b>				
$L$	$L-kp$	Valence band parameter	$\begin{cases} x = 0.0 & -6.53 & -12.947 \\ x = 0.1 & -6.79885 & -12.947 \\ x = 0.2 & -7.17333 & -12.947 \\ x = 0.3 & -7.80676 & -12.947 \\ x = 0.4 & -8.69912 & -12.947 \\ x = 0.5 & -9.85043 & -12.947 \\ x = 0.6 & -11.26068 & -12.947 \\ x = 0.7 & -12.92986 & -12.947 \\ x = 0.8 & -14.85799 & -12.947 \\ x = 0.9 & -19.11 & -12.947 \\ x = 1.0 & -31.58 & -424.00 \end{cases}$	$\hbar^2/2m$

## Chapter 22: Silicon Germanium Binary Alloy Material Model

### Valence Band Model

Table 481 Parameters of valence band container model (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$M$	$M\text{-kp}$	Valence band parameter	$\begin{cases} x = 0.0 & -4.64 \quad -0.20628 \\ x = 0.1 & -4.66253 \quad -0.20628 \\ x = 0.2 & -4.69509 \quad -0.20628 \\ x = 0.3 & -4.73278 \quad -0.20628 \\ x = 0.4 & -4.77259 \quad -0.20628 \\ x = 0.5 & -4.81753 \quad -0.20628 \\ x = 0.6 & -4.86659 \quad -0.20628 \\ x = 0.7 & -4.91977 \quad -0.20628 \\ x = 0.8 & -4.97709 \quad -0.20628 \\ x = 0.9 & -5.03853 \quad -0.20628 \\ x = 1.0 & -5.1 \quad -0.20628 \end{cases}$	$\hbar^2/2m$
$N$	$N\text{-kp}$	Valence band parameter	$\begin{cases} x = 0.0 & -8.32 \quad -12.739 \\ x = 0.1 & -8.58962 \quad -12.739 \\ x = 0.2 & -8.96483 \quad -12.739 \\ x = 0.3 & -9.59481 \quad -12.739 \\ x = 0.4 & -10.47957 \quad -12.739 \\ x = 0.5 & -11.61911 \quad -12.739 \\ x = 0.6 & -13.01344 \quad -12.739 \\ x = 0.7 & -14.66254 \quad -12.739 \\ x = 0.8 & -16.56642 \quad -12.739 \\ x = 0.9 & -20.71 \quad -12.739 \\ x = 1.0 & -32.1 \quad -375.00 \end{cases}$	$\hbar^2/2m$
$l$	$l\text{-defpot}$	Valence deformation potential	$\begin{cases} x = 0.0 & -2.3 \\ x = 1.0 & -2.4 \end{cases}$	eV
$m$	$m\text{-defpot}$	Valence deformation potential	$\begin{cases} x = 0.0 & 4.3 \\ x = 1.0 & 4.2 \end{cases}$	eV
$n$	$n\text{-defpot}$	Valence deformation potential	$\begin{cases} x = 0.0 & -9.18 \\ x = 1.0 & -7.621 \end{cases}$	eV

## Chapter 22: Silicon Germanium Binary Alloy Material Model

### Valence Band Model

Table 481 Parameters of valence band container model (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$\Delta_{\text{ss0}}$	dsso	Spin-orbit split energy	$\begin{cases} x = 0.0 & 0.0440 \\ x = 0.1 & 0.0692 \\ x = 0.2 & 0.0944 \\ x = 0.3 & 0.1196 \\ x = 0.4 & 0.1448 \\ x = 0.5 & 0.1700 \\ x = 0.6 & 0.1952 \\ x = 0.7 & 0.2204 \\ x = 0.8 & 0.2456 \\ x = 0.9 & 0.2708 \\ x = 1.0 & 0.2960 \end{cases}$	eV

To change the default parameter values of the valence bands in the container model, listed in [Table 482](#), use the following input file syntax:

```
MATERIAL SiliconGermanium.valence.<band>.<parameter> <value>
```

Table 482 Parameters of valence band model

Parameter symbol	Parameter name	Description	Default	Unit
<b>Heavy hole (HH) band</b>				
E	E	Valence band energy with respect to container energy	0.0	eV
model				
	model	Model used for transport in this band	6kp	—
<b>Light hole (LH) band</b>				
E	E	Valence band energy with respect to container energy	0.0	eV
model				
	model	Model used for transport in this band	6kp	—

## Chapter 22: Silicon Germanium Binary Alloy Material Model

### Valence Band Model

Table 482 Parameters of valence band model (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
<b>Spin split-off (SSO) band</b>				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	$\begin{cases} x = 0.0 & 0.04400 \quad 0.012 \\ x = 0.1 & 0.06812 \quad 0.012 \\ x = 0.2 & 0.09248 \quad 0.012 \\ x = 0.3 & 0.11708 \quad 0.012 \\ x = 0.4 & 0.14192 \quad 0.012 \\ x = 0.5 & 0.16700 \quad 0.012 \\ x = 0.6 & 0.19232 \quad 0.012 \\ x = 0.7 & 0.21788 \quad 0.012 \\ x = 0.8 & 0.24368 \quad 0.012 \\ x = 0.9 & 0.26972 \quad 0.012 \\ x = 1.0 & 0.29600 \quad 0.012 \end{cases}$	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	6kp	—

## Mobility Models

The valence band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models together with some phenomenological enhancement factors.

### Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 483](#), use the following input file syntax:

```
MATERIAL SiliconGermanium.valence.constant.<parameter> <value>
```

*Table 483 Parameters of constant mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	$\left\{ \begin{array}{l} x = 0.1 \ 364 \\ x = 0.2 \ 300 \\ x = 0.3 \ 300 \\ x = 0.4 \ 320 \\ x = 0.5 \ 364 \\ x = 0.6 \ 550 \\ x = 0.7 \ 700 \\ x = 0.8 \ 900 \\ x = 0.9 \ 1300 \end{array} \right.$	$\text{cm}^2/\text{Vs}$
$\zeta$	zeta	Fitting parameter	$\left\{ \begin{array}{l} x = 0.1 \ 2.21 \\ x = 0.2 \ 2.22 \\ x = 0.3 \ 2.23 \\ x = 0.4 \ 2.24 \\ x = 0.5 \ 2.25 \\ x = 0.6 \ 2.26 \\ x = 0.7 \ 2.27 \\ x = 0.8 \ 2.28 \\ x = 0.9 \ 2.29 \end{array} \right.$	—

## Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 484](#), use the following input file syntax:

```
MATERIAL SiliconGermanium.valence.Arora.<parameter> <value>
```

**Chapter 22: Silicon Germanium Binary Alloy Material Model**  
**Valence Band Model**

*Table 484 Parameters of Arora mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\max}$	mumax	Maximum mobility	$\begin{cases} x = 0.1 & 364 \\ x = 0.2 & 300 \\ x = 0.3 & 300 \\ x = 0.4 & 320 \\ x = 0.5 & 364 \\ x = 0.6 & 550 \\ x = 0.7 & 700 \\ x = 0.8 & 900 \\ x = 0.9 & 1300 \end{cases}$	$\text{cm}^2/\text{Vs}$
$\mu_{\min}$	mumin	Minimum mobility	54.3	$\text{cm}^2/\text{Vs}$
$N_0$	n0	Reference concentration	$2.35 \times 10^{17}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.88	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.33	—
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

## Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 485](#), use the following input file syntax:

```
MATERIAL SiliconGermanium.valence.Masetti.<parameter> <value>
```

**Chapter 22: Silicon Germanium Binary Alloy Material Model**  
**Valence Band Model**

*Table 485 Parameters of Masetti mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\max}$	mumax	Maximum mobility	$\begin{cases} x = 0.1 & 364 \\ x = 0.2 & 300 \\ x = 0.3 & 300 \\ x = 0.4 & 320 \\ x = 0.5 & 364 \\ x = 0.6 & 550 \\ x = 0.7 & 700 \\ x = 0.8 & 900 \\ x = 0.9 & 1300 \end{cases}$	$\text{cm}^2/\text{Vs}$
$\mu_{\min1}$	mumin1	Minimum mobility	44.9	$\text{cm}^2/\text{Vs}$
$\mu_{\min2}$	mumin2	Minimum mobility	0.0	$\text{cm}^2/\text{Vs}$
$\mu_1$	mul	Maximum mobility	29.0	$\text{cm}^2/\text{Vs}$
$C_r$	cr	Reference concentration	$2.23 \times 10^{17}$	$\text{cm}^{-3}$
$C_s$	cs	Reference solid solubility concentration	$6.10 \times 10^{20}$	$\text{cm}^{-3}$
$p_c$	pc	Fitting parameter	$9.23 \times 10^{16}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.719	—
$\beta$	beta	Fitting parameter	2.0	—
$\zeta$	zeta	Fitting parameter	$\begin{cases} x = 0.1 & 2.21 \\ x = 0.2 & 2.22 \\ x = 0.3 & 2.23 \\ x = 0.4 & 2.24 \\ x = 0.5 & 2.25 \\ x = 0.6 & 2.26 \\ x = 0.7 & 2.27 \\ x = 0.8 & 2.28 \\ x = 0.9 & 2.29 \end{cases}$	—

## Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 486](#), use the following input file syntax:

```
MATERIAL SiliconGermanium.valence.Yamaguchi.<parameter> <value>
```

*Table 486 Parameters of Yamaguchi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

## Perpendicular Field: Lombardi Mobility Model

To change the default parameter values of the Lombardi mobility model, listed in [Table 487](#), use the following input file syntax:

```
MATERIAL SiliconGermanium.valence.Lombardi.<parameter> <value>
```

*Table 487 Parameters of Lombardi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$A$	a	Fitting parameter	2.0	—
$B$	b	Fitting parameter	$9.925 \times 10^6$	cm/s
$C$	c	Fitting parameter	$2.947 \times 10^3$	$\text{cm}^{5/3} \text{V}^{-2/3} \text{s}^{-1}$
$\alpha$	alpha	Fitting parameter	0.0	$\text{cm}^3$
$\delta$	delta	Fitting parameter	$2.0546 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$2.0546 \times 10^{30}$	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	1.0	—
$\lambda$	lambda	Fitting parameter	0.0317	—
$\nu$	nu	Fitting parameter	1.0	—

**Chapter 22: Silicon Germanium Binary Alloy Material Model**  
**Valence Band Model**

*Table 487 Parameters of Lombardi mobility model (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$N_0$	n0	Fitting parameter	1.0	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	1.0	$\text{cm}^{-3}$
$l_{\text{crit}}$	lcrit	Critical length	$1 \times 10^{-6}$	cm

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in [Table 488](#), use the following input file syntax:

```
MATERIAL SiliconGermanium.valence.Caughey.<parameter> <value>
```

*Table 488 Parameters of Caughey–Thomas mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$8.37 \times 10^6$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	0.52	–
$\beta_0$	beta0	Fitting parameter	1.213	–
$\beta_{\text{exp}}$	bexp	Fitting parameter	0.17	–
$\alpha$	alpha	Fitting parameter	1.0	–

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 489](#). To change the default mobility model, use the following input file syntax:

```
MATERIAL SiliconGermanium.valence.mobility.<model> <value>
```

## Chapter 22: Silicon Germanium Binary Alloy Material Model

### Valence Band Model

Table 489 Parameters of default mobility model

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley valence band model consists of the valley minima listed in [Table 490](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL SiliconGermanium.valence.<band>.<valley> REMOVE
```

### Note:

The valence band analytic valley approximation is used only as a way to define density-of-states for drift-diffusion simulations and to define the valley minima in response to stress.

Table 490 Names of valence band minima

Valence band minima	Band name	Valley name
Heavy hole	HH	vhh
Light hole	LH	vlh
Spin split-off	SSO	vsso

## Position and Orientation

Valley minima differ in their position and orientation, the default values of which are shown in [Table 491](#). To change the default values, use the following input file syntax:

```
MATERIAL SiliconGermanium.valence.<band>.<valley>.min.<parameter> <value>
```

**Chapter 22: Silicon Germanium Binary Alloy Material Model**  
**Valence Band Model**

*Table 491 Position and orientation parameters of HH, LH, and SSO valley minima*

Parameter symbol	Parameter name	Description	Default	Unit
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.0	$2\pi/a$
$x$	x	Orientation of the x-axis	1 0 0	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	0 1 0	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	0 0 1	$\langle hkl \rangle$

## Parameters

To change the valley minima model parameters, listed in [Table 492](#), for each valley listed in [Table 490](#), use the following input file syntax:

```
MATERIAL SiliconGermanium.valence.<band>.<valley>.<parameter> <value>
```

*Table 492 Parameters of valence band minima*

Parameter symbol	Parameter name	Description	Default	Unit
<b>Heavy hole (HH) band</b>				
$E$	E	Minima energy with respect to band edge	0.0	eV
$m_x$	mx	Longitudinal effective mass	$\begin{cases} x = 0.0 & 0.9890 \\ x = 0.1 & 0.9254 \\ x = 0.2 & 0.8618 \\ x = 0.3 & 0.7982 \\ x = 0.4 & 0.7346 \\ x = 0.5 & 0.6710 \\ x = 0.6 & 0.6074 \\ x = 0.7 & 0.5438 \\ x = 0.8 & 0.4802 \\ x = 0.9 & 0.4166 \\ x = 1.0 & 0.3530 \end{cases}$	$m_e$

**Chapter 22: Silicon Germanium Binary Alloy Material Model**  
**Valence Band Model**

*Table 492 Parameters of valence band minima (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$m_y$	$m_y$	Transverse effective mass	{ x = 0.0 0.9890 x = 0.1 0.9254 x = 0.2 0.8618 x = 0.3 0.7982 x = 0.4 0.7346 x = 0.5 0.6710 x = 0.6 0.6074 x = 0.7 0.5438 x = 0.8 0.4802 x = 0.9 0.4166 x = 1.0 0.3530}	$m_e$
$m_z$	$m_z$	Transverse effective mass	{ x = 0.0 0.9890 x = 0.1 0.9254 x = 0.2 0.8618 x = 0.3 0.7982 x = 0.4 0.7346 x = 0.5 0.6710 x = 0.6 0.6074 x = 0.7 0.5438 x = 0.8 0.4802 x = 0.9 0.4166 x = 1.0 0.3530}	$m_e$
$\alpha$	$\alpha$	Valley nonparabolicity factor	0.0	—
$a_v$	$a_v$	Hydrostatic deformation potential	{ x = 0.0 2.1 x = 1.0 2.0}	eV
<b>Light hole (LH) band</b>				
$E$	$E$	Minima energy with respect to band edge	0.0	eV

**Chapter 22: Silicon Germanium Binary Alloy Material Model**  
**Valence Band Model**

*Table 492 Parameters of valence band minima (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$m_x$	<code>mx</code>	Longitudinal effective mass	{ $x = 0.0 \quad 0.9890$ $x = 0.1 \quad 0.9254$ $x = 0.2 \quad 0.8618$ $x = 0.3 \quad 0.7982$ $x = 0.4 \quad 0.7346$ $x = 0.5 \quad 0.6710$ $x = 0.6 \quad 0.6074$ $x = 0.7 \quad 0.5438$ $x = 0.8 \quad 0.4802$ $x = 0.9 \quad 0.4166$ $x = 1.0 \quad 0.3530$	$m_e$
$m_y$	<code>my</code>	Transverse effective mass	{ $x = 0.0 \quad 0.9890$ $x = 0.1 \quad 0.9254$ $x = 0.2 \quad 0.8618$ $x = 0.3 \quad 0.7982$ $x = 0.4 \quad 0.7346$ $x = 0.5 \quad 0.6710$ $x = 0.6 \quad 0.6074$ $x = 0.7 \quad 0.5438$ $x = 0.8 \quad 0.4802$ $x = 0.9 \quad 0.4166$ $x = 1.0 \quad 0.3530$	$m_e$
$m_z$	<code>mz</code>	Transverse effective mass	{ $x = 0.0 \quad 0.9890$ $x = 0.1 \quad 0.9254$ $x = 0.2 \quad 0.8618$ $x = 0.3 \quad 0.7982$ $x = 0.4 \quad 0.7346$ $x = 0.5 \quad 0.6710$ $x = 0.6 \quad 0.6074$ $x = 0.7 \quad 0.5438$ $x = 0.8 \quad 0.4802$ $x = 0.9 \quad 0.4166$ $x = 1.0 \quad 0.3530$	$m_e$

**Chapter 22: Silicon Germanium Binary Alloy Material Model**  
**Valence Band Model**

*Table 492 Parameters of valence band minima (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$\alpha$	$\alpha$	Valley nonparabolicity factor	0.0	—
$a_v$	$a_v$	Hydrostatic deformation potential	$\begin{cases} x = 0.0 & 2.1 \\ x = 1.0 & 2.0 \end{cases}$	eV
<b>Spin split-off (SSO) band</b>				
$E$	$E$	Minima energy with respect to band edge	0.0	eV
$m_x$	$m_x$	Longitudinal effective mass	$\begin{cases} x = 0.0 & 0.9890 \\ x = 0.1 & 0.9254 \\ x = 0.2 & 0.8618 \\ x = 0.3 & 0.7982 \\ x = 0.4 & 0.7346 \\ x = 0.5 & 0.6710 \\ x = 0.6 & 0.6074 \\ x = 0.7 & 0.5438 \\ x = 0.8 & 0.4802 \\ x = 0.9 & 0.4166 \\ x = 1.0 & 0.3530 \end{cases}$	$m_e$
$m_y$	$m_y$	Transverse effective mass	$\begin{cases} x = 0.0 & 0.9890 \\ x = 0.1 & 0.9254 \\ x = 0.2 & 0.8618 \\ x = 0.3 & 0.7982 \\ x = 0.4 & 0.7346 \\ x = 0.5 & 0.6710 \\ x = 0.6 & 0.6074 \\ x = 0.7 & 0.5438 \\ x = 0.8 & 0.4802 \\ x = 0.9 & 0.4166 \\ x = 1.0 & 0.3530 \end{cases}$	$m_e$

## Chapter 22: Silicon Germanium Binary Alloy Material Model

### Valence Band Model

Table 492 Parameters of valence band minima (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$m_z$	$mz$	Transverse effective mass	$\begin{cases} x = 0.0 & 0.9890 \\ x = 0.1 & 0.9254 \\ x = 0.2 & 0.8618 \\ x = 0.3 & 0.7982 \\ x = 0.4 & 0.7346 \\ x = 0.5 & 0.6710 \\ x = 0.6 & 0.6074 \\ x = 0.7 & 0.5438 \\ x = 0.8 & 0.4802 \\ x = 0.9 & 0.4166 \\ x = 1.0 & 0.3530 \end{cases}$	$m_e$
$\alpha$	$\alpha$	Valley nonparabolicity factor	0.0	—
$a_v$	$av$	Hydrostatic deformation potential	$\begin{cases} x = 0.0 & 2.1 \\ x = 1.0 & 2.0 \end{cases}$	eV

## Heavy-Hole Band Scattering Mechanisms

The heavy-hole (HH) defines a set of scattering mechanisms that is consistent with both the silicon and germanium definitions. By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL SiliconGermanium.valence.HH.vhh.<mechanism> ADD
```

```
MATERIAL SiliconGermanium.valence.HH.vhh.<mechanism> REMOVE
```

## Parameters of Scattering Mechanisms

To change parameter values, use the following input file syntax:

```
MATERIAL SiliconGermanium.valence.HH.vhh.<mechanism>.<parameter> <value>
```

### Inelastic Acoustic Phonon Scattering

Both silicon and germanium phonon modes are included for SiGe. In each case, the squared deformation potential is weighted by the mole fraction,  $x$  (germanium modes) or  $1-x$  (silicon modes).

The default parameter values of intravalley acoustic phonon scattering are consistent with the values used for silicon (see [Table 125 on page 425](#)) and germanium (see [Table 190 on page 473](#)).

### Optical Phonon Scattering

Both silicon and germanium phonon modes are included for SiGe. In each case, the squared coupling constant is weighted by the mole fraction,  $x$  (germanium modes) or  $1-x$  (silicon modes).

The default parameter values of optical phonon scattering are consistent with the values used for silicon (see [Table 126 on page 425](#)) and germanium (see [Table 191 on page 474](#)).

### Alloy Potential Scattering

[Table 493](#) lists the default parameter values of intravalley alloy potential scattering.

*Table 493 Parameters of alloy potential scattering*

Parameter symbol	Parameter name	Valley name:	HH	Unit
		Mechanism name:	al	
		Description	Default	
$U$	$U$	Alloy potential	1.7	eV
$i$	final	Final minima	HH	—

---

### Light-Hole Band Scattering Mechanisms

The light-hole (LH) defines a set of scattering mechanisms that is consistent with both the silicon and germanium definitions. By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL SiliconGermanium.valence.LH.vlh.<mechanism> ADD
```

```
MATERIAL SiliconGermanium.valence.LH.vlh.<mechanism> REMOVE
```

## Parameters of Scattering Mechanisms

To change parameter values, use the following input file syntax:

```
MATERIAL SiliconGermanium.valence.LH.vlh.<mechanism>.<parameter> <value>
```

### Inelastic Acoustic Phonon Scattering

Both silicon and germanium phonon modes are included for SiGe. In each case, the squared deformation potential is weighted by the mole fraction,  $x$  (germanium modes) or  $1-x$  (silicon modes).

The default parameter values of intravalley acoustic phonon scattering are consistent with the values used for silicon (see [Table 128 on page 426](#)) and germanium (see [Table 193 on page 475](#)).

### Optical Phonon Scattering

Both silicon and germanium phonon modes are included for SiGe. In each case, the squared coupling constant is weighted by the mole fraction,  $x$  (germanium modes) or  $1-x$  (silicon modes).

The default parameter values of optical phonon scattering are consistent with the values used for silicon (see [Table 129 on page 427](#)) and germanium (see [Table 194 on page 476](#)).

### Alloy Potential Scattering

[Table 494](#) lists the default parameter values of intravalley alloy potential scattering.

*Table 494 Parameters of alloy potential scattering*

Parameter symbol	Parameter name	Valley name:	LH	Unit
		Mechanism name:	al	
		Description	Default	
$U$	$U$	Alloy potential	1.7	eV
$i$	final	Final minima	LH	-

## Spin Split-Off Band Scattering Mechanisms

The spin split-off (SSO) defines a set of scattering mechanisms that is consistent with both the silicon and germanium definitions. By default, all these scattering mechanisms are added to the default scattering model.

## Chapter 22: Silicon Germanium Binary Alloy Material Model

### Valence Band Model

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL SiliconGermanium.valence.SSO.vssO.<mechanism> ADD
```

```
MATERIAL SiliconGermanium.valence.SSO.vssO.<mechanism> REMOVE
```

## Parameters of Scattering Mechanisms

To change parameter values, use the following input file syntax:

```
MATERIAL SiliconGermanium.valence.SSO.vssO.<mechanism>.<parameter> <value>
```

### Inelastic Acoustic Phonon Scattering

Both silicon and germanium phonon modes are included for SiGe. In each case, the squared deformation potential is weighted by the mole fraction,  $x$  (germanium modes) or  $1-x$  (silicon modes).

The default parameter values of intravalley acoustic phonon scattering are consistent with the values used for silicon (see [Table 131 on page 428](#)) and germanium (see [Table 196 on page 477](#)).

### Optical Phonon Scattering

Both silicon and germanium phonon modes are included for SiGe. In each case, the squared coupling constant is weighted by the mole fraction,  $x$  (germanium modes) or  $1-x$  (silicon modes).

The default parameter values of optical phonon scattering are consistent with the values used for silicon (see [Table 132 on page 429](#)) and germanium (see [Table 197 on page 478](#)).

### Alloy Potential Scattering

[Table 495](#) lists the default parameter values of intravalley alloy potential scattering.

*Table 495 Parameters of alloy potential scattering*

Parameter symbol	Parameter name	Valley name:	SSO	Unit
		Mechanism name:	al	
		Description	Default	
$U$	$U$	Alloy potential	1.7	eV
$i$	final	Final minima	SSO	-

---

## Ionized Impurity Scattering

Ionized impurity scattering is defined for each valley in a valence band and is treated as an intravalley process by default, so that the final valley after scattering is the same as the initial valley.

*Table 496 Parameters of ionized impurity scattering*

Parameter symbol	Parameter name	Valley name:	All valleys	Unit
		Mechanism name:	II	
		Description	Default	
<i>i</i>	final	Final minimum	Same as initial minimum	–

## Ionized Impurity Empirical Rate Factor

The ionized impurity scattering model includes a scaling factor for the empirical correction of the calculated scattering rate as a function of doping density.

To redefine the default empirical factor, use the following input file syntax:

```
MATERIAL SiliconGermanium.valence.IIfac N <Nvalue> [<Nvalue2>] <rule>
<value>
```

Here, **IIfac** is a piecewise interpolation parameter that defines a correction factor **<value>** for a value **<Nvalue>** of the doping concentration **N**. The interpolation model used to return values between specified densities is given by **<rule>**, which might require an upper bound of the density [**<Nvalue2>**]. For a description of the interpolation parameter type, see [Interpolation Methods on page 301](#).

By default, the empirical correction for ionized impurity is 1.0. However, for holes in the material, a non-unity default value is provided to best match experimental low-field concentration-dependent mobility.

---

## Surface Roughness Scattering

[Table 497](#) lists the default parameter values of surface roughness scattering. These parameters apply to all valleys and to all equivalent surface orientations.

*Table 497 Parameters of surface roughness scattering*

Parameter symbol	Parameter name	Mechanism name:	SR		Unit
		Description	Default		
$\Delta$	rms	RMS amplitude	0.70	0.10	nm
$L_c$	l	Correlation length	2.00	0.30	nm
$\langle hkl \rangle$	orient	Surface orientation	(001)	(110)	–
$i$	carrier	Carrier type	holes	holes	–

---

## Remote Coulomb Scattering

[Table 498](#) lists the default parameter values of remote Coulomb scattering, which is treated as an intravalley process. These parameters apply to all valleys.

*Table 498 Parameters of remote Coulomb scattering*

Parameter symbol	Parameter name	Mechanism name:	RC		Unit
		Description	Default		
$z_d$	zd	Depth of charge centroid	1.5		nm
$E_0$	e0	Minimum energy for tabulating rate	0		eV
$N_0$	n0	Minimum screening density	$5 \times 10^{15}$		$\text{cm}^{-3}$
$i$	final	Final minimum	Same as initial minimum		–

To define the interface charge density for remote Coulomb scattering, follow the descriptions in [Defining Interface Models on page 217](#). By default, no interface charge is applied.

## Indium Gallium Arsenide Binary Alloy Material Model

---

*This chapter describes the  $In_{1-x}Ga_xAs$  binary alloy material model.*

---

### Bulk Material Model

This section describes the bulk material model for the  $In_{1-x}Ga_xAs$  binary alloy material.

---

### Parameters of Bulk Material Model

To change the default parameter values in [Table 499](#), use the following input file syntax:

```
MATERIAL InGaAs.<parameter> <value>
```

*Table 499 Bulk material model parameters*

Parameter symbol	Parameter name	Description	Interpolation	Default	Unit
<b>Binary material-specific properties</b>					
$x$	x_fraction	Binary alloy fraction	NA	—	—
$A_{1-x}$	material1	Binary alloy constituent material <i>A</i>	NA	InAs	—
$B_x$	material2	Binary alloy constituent material <i>B</i>	NA	GaAs	—
<b>Crystal lattice and orientation in simulation domain</b>					
$ a $	a	Magnitude of lattice vector <i>a</i>	linear	—	Å
$ b $	b	Magnitude of lattice vector <i>b</i>	linear	—	Å

**Chapter 23: Indium Gallium Arsenide Binary Alloy Material Model**  
**Bulk Material Model**

*Table 499 Bulk material model parameters (Continued)*

Parameter symbol	Parameter name	Description	Interpolation	Default	Unit
$ c $	c	Magnitude of lattice vector $c$	linear	—	Å
$\alpha$	alpha	Angle between $b$ and $c$	NA	90	degree
$\beta$	beta	Angle between $c$ and $a$	NA	90	degree
$\gamma$	gamma	Angle between $a$ and $b$	NA	90	degree
$\langle hkl \rangle_x$	x	Orientation in the x-direction	NA	1 0 0	—
$\langle hkl \rangle_z$	z	Orientation in the z-direction	NA	0 0 1	—
<b>Bulk electrical and mechanical properties</b>					
$\kappa$	permittivity	Relative dielectric constant	linear	—	—
$\kappa_\infty$	k_inf	High-frequency permittivity	linear	—	—
$\rho$	density	Mass density	linear	—	g/cm <sup>3</sup>
$C_{11}$	C11	Elastic stiffness matrix element	linear	—	GPa
$C_{12}$	C12	Elastic stiffness matrix element	linear	—	GPa
$C_{44}$	C44	Elastic stiffness matrix element	linear	—	GPa

## Band-to-Band Tunneling Parameters

To change the default parameter values for the Kane model, listed in [Table 500](#), use the following input file syntax:

```
MATERIAL InGaAs.BTBT.<parameter> <value>
```

**Chapter 23: Indium Gallium Arsenide Binary Alloy Material Model**  
 Conduction Band Model

*Table 500 Band-to-band tunneling parameters*

Parameter symbol	Parameter name	Description	Default	Unit
$D_{TA}$	DTA	Acoustic phonon deformation potential	0.0	eV
$\epsilon_{TA}$	epsilonTA	Acoustic phonon energy	0.0	eV

## Conduction Band Model

This section describes the conduction band model.

### Band Edge Parameters

To change the default parameter values of the conduction band container model, listed in [Table 501](#), use the following input file syntax:

```
MATERIAL InGaAs.conduction.<parameter> <value>
```

*Table 501 Parameters of conduction band container model*

Parameter symbol	Parameter name	Description	Interpolation	Default	Unit
$E$	E	Conduction band energy with respect to vacuum	linear	4.485	eV
$m_{dg_x}$	dgx	Electron density gradient effective x-mass	constant	0.3	$m_e$
$m_{dg_y}$	dgy	Electron density gradient effective y-mass	constant	0.3	$m_e$
$m_{dg_z}$	dgz	Electron density gradient effective z-mass	constant	0.3	$m_e$

To change the default parameter values of the conduction bands in the container model, listed in [Table 502](#), use the following input file syntax:

```
MATERIAL InGaAs.conduction.<band>.<parameter> <value>
```

## Chapter 23: Indium Gallium Arsenide Binary Alloy Material Model

### Conduction Band Model

*Table 502 Parameters of conduction band model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	<code>E</code>	Conduction band energy with respect to container energy	0.0	eV
$model$	<code>model</code>	Model used for transport in this band	<code>ema</code>	—

## Mobility Models

The conduction band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models.

### Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 503](#), use the following input file syntax:

```
MATERIAL InGaAs.conduction.constant.<parameter> <value>
```

*Table 503 Parameters of constant mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	<code>mu0</code>	Constant low-field mobility	$\begin{cases} x = 0.0 & 3.4 \times 10^4 \\ x = 0.47 & 1.4 \times 10^4 \\ x = 1.0 & 9.4 \times 10^3 \end{cases}$	$\text{cm}^2/\text{Vs}$
$\zeta$	<code>zeta</code>	Fitting parameter	2.1	—

### Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 504](#), use the following input file syntax:

```
MATERIAL InGaAs.conduction.Arora.<parameter> <value>
```

**Chapter 23: Indium Gallium Arsenide Binary Alloy Material Model**  
 Conduction Band Model

*Table 504 Parameters of Arora mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\max}$	mumax	Maximum mobility	$\begin{cases} x = 0.0 & 3.4 \times 10^4 \\ x = 0.47 & 1.4 \times 10^4 \\ x = 1.0 & 9.4 \times 10^3 \end{cases}$	cm <sup>2</sup> /Vs
$\mu_{\min}$	mumin	Minimum mobility	88.0	cm <sup>2</sup> /Vs
$N_0$	n0	Reference concentration	$1.25 \times 10^{17}$	cm <sup>-3</sup>
$\alpha$	alpha	Fitting parameter	0.88	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.33	—
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

### Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 505](#), use the following input file syntax:

```
MATERIAL InGaAs.conduction.Masetti.<parameter> <value>
```

*Table 505 Parameters of Masetti mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\max}$	mumax	Maximum mobility	$\begin{cases} x = 0.0 & 3.4 \times 10^4 \\ x = 0.47 & 1.4 \times 10^4 \\ x = 1.0 & 9.4 \times 10^3 \end{cases}$	cm <sup>2</sup> /Vs

**Chapter 23: Indium Gallium Arsenide Binary Alloy Material Model**  
 Conduction Band Model

*Table 505 Parameters of Masetti mobility model (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min 1}$	mumin1	Minimum mobility	220.0	$\text{cm}^2/\text{Vs}$
$\mu_{\min 2}$	mumin2	Minimum mobility	220.0	$\text{cm}^2/\text{Vs}$
$\mu_1$	mul	Maximum mobility	1.0	$\text{cm}^2/\text{Vs}$
$C_r$	cr	Reference concentration	$1.2 \times 10^{17}$	$\text{cm}^{-3}$
$C_s$	cs	Reference solid solubility concentration	0.0	$\text{cm}^{-3}$
$p_c$	pc	Fitting parameter	0.0	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.5	—
$\beta$	beta	Fitting parameter	2.0	—
$\zeta$	zeta	Fitting parameter	2.5	—

## Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 506](#), use the following input file syntax:

```
MATERIAL InGaAs.conduction.Yamaguchi.<parameter> <value>
```

*Table 506 Parameters of Yamaguchi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

## Perpendicular Field: Lombardi Mobility Model

To change the default parameter values of the Lombardi mobility model, listed in [Table 507](#), use the following input file syntax:

```
MATERIAL InGaAs.conduction.Lombardi.<parameter> <value>
```

*Table 507 Parameters of Lombardi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
A	a	Fitting parameter	2.0	—
B	b	Fitting parameter	$4.75 \times 10^7$	cm/s
C	c	Fitting parameter	$5.80 \times 10^2$	$\text{cm}^{5/3} \text{V}^{-2/3} \text{s}^{-1}$
$\alpha$	alpha	Fitting parameter	0.0	$\text{cm}^3$
$\delta$	delta	Fitting parameter	$5.82 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$5.82 \times 10^{30}$	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	1.0	—
$\lambda$	lambda	Fitting parameter	0.125	—
$\nu$	nu	Fitting parameter	1.0	—
$N_0$	n0	Fitting parameter	1.0	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	1.0	$\text{cm}^{-3}$
$l_{\text{crit}}$	lcrit	Critical length	$1 \times 10^{-6}$	cm

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in [Table 508](#), use the following input file syntax:

```
MATERIAL InGaAs.conduction.Caughey.<parameter> <value>
```

**Chapter 23: Indium Gallium Arsenide Binary Alloy Material Model**  
 Conduction Band Model

*Table 508 Parameters of Caughey–Thomas mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$6.0 \times 10^6$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	0.87	—
$\beta_0$	beta0	Fitting parameter	1.109	—
$\beta_{\text{exp}}$	bexp	Fitting parameter	0.66	—
$\alpha$	alpha	Fitting parameter	0.0	—

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 509](#).

To change the default mobility model, use the following input file syntax:

```
MATERIAL InGaAs.conduction.mobility.<model> <value>
```

*Table 509 Parameters of default mobility model*

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley conduction band model consists of the valley minima listed in [Table 510](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL InGaAs.conduction.<band>.<valley> REMOVE
```

**Chapter 23: Indium Gallium Arsenide Binary Alloy Material Model**  
 Conduction Band Model

*Table 510 Names of conduction band C1 minima*

Conduction band minimum	Valley name
X	X1, X2, X3, X4, X5, X6
L	L1, L2, L3, L4, L5, L6, L7, L8
$\Gamma$	G

## Position and Orientation

Valley minima differ in their position and orientation, the default values of which are shown in [Table 511](#), [Table 512](#), and [Table 513](#).

To change default values, use the following input file syntax:

```
MATERIAL InGaAs.conduction.C1.<valley>.min.<parameter> <value>
```

*Table 511 Position and orientation parameters of L-minima of conduction band*

Parameter symbol	Parameter name	Description	Interpolation	Unit
<b>L1</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
x	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
y	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
z	z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>L2</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
x	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
y	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
z	z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$

**Chapter 23: Indium Gallium Arsenide Binary Alloy Material Model**  
 Conduction Band Model

*Table 511 Position and orientation parameters of L-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Interpolation	Unit
<b>L3</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>L4</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>L5</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>L6</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$

**Chapter 23: Indium Gallium Arsenide Binary Alloy Material Model**  
 Conduction Band Model

*Table 511 Position and orientation parameters of L-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Interpolation	Unit
$z$	$z$	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>L7</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	$x$	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	$y$	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	$z$	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>L8</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	$x$	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	$y$	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	$z$	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$

*Table 512 Position and orientation parameters of  $\Gamma$ -minimum of conduction band*

Parameter symbol	Parameter name	Description	Interpolation	Unit
<b>G</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	$x$	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	$y$	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	$z$	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$

**Chapter 23: Indium Gallium Arsenide Binary Alloy Material Model**  
 Conduction Band Model

*Table 513 Position and orientation parameters of X-minima of conduction band*

Parameter symbol	Parameter name	Description	Interpolation	Unit
<b>X1</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>X2</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>X3</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>X4</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$

**Chapter 23: Indium Gallium Arsenide Binary Alloy Material Model**  
 Conduction Band Model

*Table 513 Position and orientation parameters of X-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Interpolation	Unit
y	Y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>X5</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
x	X	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>X6</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
x	X	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
y	Y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
z	Z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$

## Parameters

To change the default parameter values of the valley minima models, listed in the following tables, for each valley listed in [Table 510](#), use the following input file syntax:

```
MATERIAL InGaAs.conduction.C1.<valley>.<parameter> <value>
```

### Note:

By default, all  $X$ -minima have the same parameter values, and all  $L$ -minima have the same parameter values.

**Chapter 23: Indium Gallium Arsenide Binary Alloy Material Model**  
 Conduction Band Model

*Table 514 Parameters of L-valley model*

Parameter symbol	Parameter name	Description	Interpolation	Unit
$E$	$E$	Minima with respect to band edge	quadraticIII 0.72 -0.65 0.22	eV
$m_x$	$m_x$	Longitudinal effective mass	linear	$m_e$
$m_y$	$m_y$	Transverse effective mass	linear	$m_e$
$m_z$	$m_z$	Transverse effective mass	linear	$m_e$
$\alpha$	$a$	Valley nonparabolicity factor	linear	—
$\Xi_u$	$\xi_{i\_u}$	Uniaxial deformation potential	linear	eV
$\Xi_d$	$\xi_{i\_d}$	Dilatation deformation potential	linear	eV
$\Xi'_u$	$\xi_{i\_u\_prime}$	Uniaxial mass deformation	linear	eV

*Table 515 Parameters of X-valley model*

Parameter symbol	Parameter name	Description	Interpolation	Unit
$E$	$E$	Minima with respect to band edge	quadraticIII 1.01 -1.26 0.73	eV
$m_x$	$m_x$	Longitudinal effective mass	linear	$m_e$
$m_y$	$m_y$	Transverse effective mass	linear	$m_e$
$m_z$	$m_z$	Transverse effective mass	linear	$m_e$
$\alpha$	$a$	Valley nonparabolicity factor	linear	—
$\Xi_u$	$\xi_{i\_u}$	Uniaxial deformation potential	linear	eV

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*Table 515 Parameters of X-valley model (Continued)*

Parameter symbol	Parameter name	Description	Interpolation	Unit
$\Xi_d$	$\xi_i_d$	Dilatation deformation potential	linear	eV
$\Xi'_u$	$\xi_i_u_{\text{prime}}$	Uniaxial mass deformation	linear	eV

*Table 516 Parameters of  $\Gamma$ -valley model*

Parameter symbol	Parameter name	Description	Interpolation	Unit
$E$	$E$	Minima with respect to band edge	linear	eV
$m_x$	$m_x$	Longitudinal effective mass	quadraticIII 0.023 0.037 0.003	$m_e$
$m_y$	$m_y$	Transverse effective mass	quadraticIII 0.023 0.037 0.003	$m_e$
$m_z$	$m_z$	Transverse effective mass	quadraticIII 0.023 0.037 0.003	$m_e$
$\alpha$	$a$	Valley nonparabolicity factor	linear	—
$\Xi_u$	$\xi_i_u$	Uniaxial deformation potential	linear	eV
$\Xi_d$	$\xi_i_d$	Dilatation deformation potential	linear	eV
$\Xi'_u$	$\xi_i_u_{\text{prime}}$	Uniaxial mass deformation	linear	eV

---

## L-Valley Scattering Mechanisms

The eight  $L$ -minima define the set of scattering mechanisms listed in [Table 517](#). By default, all these scattering mechanisms are added to the default scattering model.

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To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL InGaAs.conduction.C1.<valley>.<mechanism> ADD
```

```
MATERIAL InGaAs.conduction.C1.<valley>.<mechanism> REMOVE
```

Table 517 Scattering mechanisms for L-minima

Scattering mechanism	L1	L2	L3	L4	L5	L6	L7	L8
	Mechanism name							
Acoustic Phonon (elastic)	ac	ac	ac	ac	ac	ac	ac	ac
Polar Optical (intra)	pop	pop	pop	pop	pop	pop	pop	pop
Optical Phonon (intra)	opl	opl	opl	opl	opl	opl	opl	opl
Optical Phonon (inter)	opl2	opl1						
Optical Phonon (inter)	opl3	opl3	opl2	opl2	opl2	opl2	opl2	opl2
Optical Phonon (inter)	opl4	opl4	opl4	opl3	opl3	opl3	opl3	opl3
Optical Phonon (inter)	opl5	opl5	opl5	opl5	opl4	opl4	opl4	opl4
Optical Phonon (inter)	opl6	opl6	opl6	opl6	opl6	opl5	opl5	opl5
Optical Phonon (inter)	opl7	opl7	opl7	opl7	opl7	opl7	opl6	opl6
Optical Phonon (inter)	opl8	opl8	opl8	opl8	opl8	opl8	opl8	opl7
Optical Phonon (inter)	opx1	opx1	opx1	opx1	opx1	opx1	opx1	opx1
Optical Phonon (inter)	opx2	opx2	opx2	opx2	opx2	opx2	opx2	opx2
Optical Phonon (inter)	opx3	opx3	opx3	opx3	opx3	opx3	opx3	opx3
Optical Phonon (inter)	opx4	opx4	opx4	opx4	opx4	opx4	opx4	opx4
Optical Phonon (inter)	opx5	opx5	opx5	opx5	opx5	opx5	opx5	opx5
Optical Phonon (inter)	opx6	opx6	opx6	opx6	opx6	opx6	opx6	opx6
Optical Phonon (inter)	opg	opg	opg	opg	opg	opg	opg	opg
Ionized Impurity	II	II	II	II	II	II	II	II

*Table 517 Scattering mechanisms for L-minima (Continued)*

Scattering mechanism	L1	L2	L3	L4	L5	L6	L7	L8
<b>Mechanism name</b>								
Surface Roughness	SR							
Remote Coulomb	RC							

## Parameter of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each *L*-minimum, listed in [Table 517](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL InGaAs.conduction.C1.<valley>.<mechanism>.<parameter> <value>
```

### Elastic Acoustic Phonon Scattering

[Table 518](#) lists the default parameter values of intravalley elastic acoustic phonon scattering.

*Table 518 Parameters of elastic acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	L[1, 2, 3, 4, 5, 6, 7, 8]	Unit
		Mechanism name:	ac	
		Description	Interpolation	
$\Delta_{ac}$	D	Acoustic deformation	linear	eV
v	v	Velocity	linear	m/s
i	final	Final minima	Set from $B_x$ material	–

### Polar-Optical Phonon Scattering

Table 519 lists the default parameter values of intravalley polar-optical phonon scattering.

Table 519 Parameters of polar-optical phonon scattering

Parameter symbol	Parameter name	Valley name:	L[1, 2, 3, 4, 5, 6, 7, 8]	Unit
		Mechanism name:	pop	
		Description	Interpolation	
$E_{op}$	E	Phonon energy	linear	eV
$i$	final	Final minima	Set from $B_x$ material	—

### Optical Phonon Scattering

Table 520 to Table 523 list the default parameter values of intravalley and intervalley optical phonon scattering.

Table 520 Parameters of intravalley optical phonon scattering

Parameter symbol	Parameter name	Valley name:	L[1, 2, 3, 4, 5, 6, 7, 8]	Unit
		Mechanism name:	opl	
		Description	Interpolation	
$E_{op}$	E	Phonon energy	linear	eV
$D_{op}$	Cc	Coupling constant	linear	eV/m
$i$	final	Final minima	Set from $B_x$ material	—

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*Table 521 Parameters of intervalley L to L optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L[1, 2, 3, 4, 5, 6, 7, 8]	Unit
		Mechanism name:	opl[1, 2, 3, 4, 5, 6, 7, 8]	
		Description	Interpolation	
$E_{op}$	E	Phonon energy	linear	eV
$D_{op}$	Cc	Coupling constant	linear	eV/m
$i$	final	Final minima	Set from $B_x$ material	–

*Table 522 Parameters of intervalley L to  $\Gamma$  optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L[1, 2, 3, 4, 5, 6, 7, 8]	Unit
		Mechanism name:	opg	
		Description	Interpolation	
$E_{op}$	E	Phonon energy	linear	eV
$D_{op}$	Cc	Coupling constant	linear	eV/m
$i$	final	Final minima	Set from $B_x$ material	–

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*Table 523 Parameters of intervalley L to X optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L[1, 2, 3, 4, 5, 6, 7, 8]	Unit
		Mechanism name:	opx[1, 2, 3, 4, 5, 6]	
		Description	Interpolation	
$E_{\text{op}}$	E	Phonon energy	linear	eV
$D_{\text{op}}$	Cc	Coupling constant	linear	eV/m
$i$	final	Final minima	Set from $B_x$ material	–

## Γ-Valley Scattering Mechanisms

The  $\Gamma$ -minimum defines the set of scattering mechanisms listed in [Table 524](#). By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL InGaAs.conduction.C2.G.<mechanism> ADD
MATERIAL InGaAs.conduction.C2.G.<mechanism> REMOVE
```

*Table 524 Scattering mechanisms for  $\Gamma$ -minimum*

Scattering mechanism	Mechanism name
Acoustic Phonon (elastic)	ac
Polar Optical (intra)	pop
Optical Phonon (inter)	opl1
Optical Phonon (inter)	opl2
Optical Phonon (inter)	opl3
Optical Phonon (inter)	opl4
Optical Phonon (inter)	opl5
Optical Phonon (inter)	opl6

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*Table 524 Scattering mechanisms for  $\Gamma$ -minimum (Continued)*

Scattering mechanism	Mechanism name
Optical Phonon (inter)	opl7
Optical Phonon (inter)	opl8
Optical Phonon (inter)	opx1
Optical Phonon (inter)	opx2
Optical Phonon (inter)	opx3
Optical Phonon (inter)	opx4
Optical Phonon (inter)	opx5
Optical Phonon (inter)	opx6
Ionized Impurity	II
Surface Roughness	SR
Remote Coulomb	RC

## Parameters of Scattering Mechanisms

To change the default parameter values of the scattering mechanisms listed in [Table 524](#), use the following input file syntax:

```
MATERIAL InGaAs.conduction.C2.G.<mechanism>.<parameter> <value>
```

### Elastic Acoustic Phonon Scattering

[Table 525](#) lists the default parameter values of intravalley elastic acoustic phonon scattering.

*Table 525 Parameters of elastic acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	ac	
		Description	Interpolation	
$\Delta_{ac}$	D	Acoustic deformation	linear	eV

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*Table 525 Parameters of elastic acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	ac	
		Description	Interpolation	
v	v	Velocity	linear	m/s
i	final	Final minima	Set from $B_x$ material	–

### Polar-Optical Phonon Scattering

[Table 526](#) lists the default parameter values of intravalley polar-optical phonon scattering.

*Table 526 Parameters of polar-optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	pop	
		Description	Interpolation	
$E_{op}$	E	Phonon energy	linear	eV
i	final	Final minima	Set from $B_x$ material	–

### Optical Phonon Scattering

[Table 527](#) and [Table 528](#) list the default parameter values of intervalley optical phonon scattering.

*Table 527 Parameters for intervalley  $\Gamma$  to L optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	opl[1, 2, 3, 4, 5, 6, 7, 8]	
		Description	Interpolation	
$E_{op}$	E	Phonon energy	linear	eV
$D_{op}$	cc	Coupling constant	linear	eV/m

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*Table 527 Parameters for intervalley  $\Gamma$  to L optical phonon scattering (Continued)*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	opl[1, 2, 3, 4, 5, 6, 7, 8]	
		Description	Interpolation	
$i$	final	Final minima	Set from $B_x$ material	–

*Table 528 Parameters for intervalley  $\Gamma$  to X optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	opx[1, 2, 3, 4, 5, 6]	
		Description	Interpolation	
$E_{\text{op}}$	E	Phonon energy	linear	eV
$D_{\text{op}}$	cc	Coupling constant	linear	eV/m
$i$	final	Final minima	Set from $B_x$ material	–

## X-Valley Scattering Mechanisms

The six X-minima define the set of scattering mechanisms listed in [Table 529](#). By default, all these scattering mechanisms are added to the default scattering model. To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL InGaAs.conduction.C1.<valley>.<mechanism> ADD
```

```
MATERIAL InGaAs.conduction.C1.<valley>.<mechanism> REMOVE
```

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*Table 529 Scattering mechanisms for X-minima*

Scattering mechanism	X1	X2	X3	X4	X5	X6
	Mechanism name					
Acoustic Phonon (elastic)	ac	ac	ac	ac	ac	ac
Polar Optical (intra)	pop	pop	pop	pop	pop	pop
Optical Phonon (inter)	opx2	opx1	opx1	opx1	opx1	opx1
Optical Phonon (inter)	opx3	opx3	opx2	opx3	opx3	opx3
Optical Phonon (inter)	opx4	opx4	opx4	opx2	opx4	opx4
Optical Phonon (inter)	opx5	opx5	opx5	opx5	opx2	opx5
Optical Phonon (inter)	opx6	opx6	opx6	opx6	opx6	opx2
Optical Phonon (inter)	opl1	opl1	opl1	opl1	opl1	opl1
Optical Phonon (inter)	opl2	opl2	opl2	opl2	opl2	opl2
Optical Phonon (inter)	opl3	opl3	opl3	opl3	opl3	opl3
Optical Phonon (inter)	opl4	opl4	opl4	opl4	opl4	opl4
Optical Phonon (inter)	opl5	opl5	opl5	opl5	opl5	opl5
Optical Phonon (inter)	opl6	opl6	opl6	opl6	opl6	opl6
Optical Phonon (inter)	opl7	opl7	opl7	opl7	opl7	opl7
Optical Phonon (inter)	opl8	opl8	opl8	opl8	opl8	opl8
Optical Phonon (inter)	opg	opg	opg	opg	opg	opg
Ionized Impurity	II	II	II	II	II	II
Surface Roughness	SR	SR	SR	SR	SR	SR
Remote Coulomb	RC	RC	RC	RC	RC	RC

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each  $X$ -minimum, listed in [Table 529](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL InGaAs.conduction.C1.<valley>.<mechanism>.<parameter> <value>
```

### Elastic Acoustic Phonon Scattering

[Table 530](#) lists the default parameter values of intravalley elastic acoustic phonon scattering.

*Table 530 Parameters of elastic acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	X[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	ac	
		Description	Interpolation	
$\Delta_{ac}$	D	Acoustic deformation	linear	eV
$v$	v	Velocity	linear	m/s
$i$	final	Final minima	Set from $B_x$ material	—

### Polar-Optical Phonon Scattering

[Table 531](#) lists the default parameter values of intravalley polar-optical phonon scattering.

*Table 531 Parameters of polar-optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	pop	
		Description	Interpolation	
$E_{op}$	E	Phonon energy	linear	eV
$i$	final	Final minima	Set from $B_x$ material	—

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### Optical Phonon Scattering

Table 532 to Table 534 list the default parameter values of intervalley optical phonon scattering.

Table 532 Parameters of intervalley X to X optical phonon scattering

Parameter symbol	Parameter name	Valley name:	X[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	opx[1, 2, 3, 4, 5, 6]	
		Description	Interpolation	
$E_{\text{op}}$	E	Phonon energy	linear	eV
$D_{\text{op}}$	cc	Coupling constant	linear	eV/m
$i$	final	Final minima	Set from $B_x$ material	—

Table 533 Parameters of intervalley X to L optical phonon scattering

Parameter symbol	Parameter name	Valley name:	X[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	opl[1, 2, 3, 4, 5, 6, 7, 8]	
		Description	Interpolation	
$E_{\text{op}}$	E	Phonon energy	linear	eV
$D_{\text{op}}$	cc	Coupling constant	linear	eV/m
$i$	final	Final minima	Set from $B_x$ material	—

*Table 534 Parameters of intervalley X to  $\Gamma$  optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	opg	
		Description	Interpolation	
$E_{\text{op}}$	E	Phonon energy	linear	eV
$D_{\text{op}}$	Cc	Coupling constant	linear	eV/m
$i$	final	Final minima	Set from $B_x$ material	—

## Ionized Impurity Scattering

Ionized impurity scattering is defined for each valley in a conduction band and is treated as an intravalley process by default, so that the final valley after scattering is the same as the initial valley.

*Table 535 Parameters of ionized impurity scattering*

Parameter symbol	Parameter name	Valley name:	All valleys	Unit
		Mechanism name:	II	
		Description	Default	
$i$	final	Final minimum	Same as initial minimum	—

## Ionized Impurity Empirical Rate Factor

The ionized impurity scattering model includes a scaling factor for the empirical correction of the calculated scattering rate as a function of doping density.

To redefine the default empirical factor, use the following input file syntax:

```
MATERIAL InGaAs.conduction.IIfac N <Nvalue> [<Nvalue2>] <rule> <value>
```

Here, **IIfac** is a piecewise interpolation parameter that defines a correction factor **<value>** for a value **<Nvalue>** of the doping concentration **N**. The interpolation model used to return values between specified densities is given by **<rule>**, which might require an upper bound

of the density [`<Nvalue2>`]. For a description of the interpolation parameter type, see [Interpolation Methods on page 301](#).

By default, the empirical correction for ionized impurity is 1.0. However, for holes in the material, a non-unity default value is provided to best match experimental low-field concentration-dependent mobility.

## Surface Roughness Scattering

[Table 536](#) lists the default parameter values of surface roughness scattering. These parameters apply to all valleys and to all equivalent surface orientations.

*Table 536 Parameters of surface roughness scattering*

Parameter symbol	Parameter name	Mechanism name:	SR	Unit
		Description		
$\Delta$	rms	RMS amplitude	1.20	nm
$L_c$	l	Correlation length	1.00	nm

## Remote Coulomb Scattering

[Table 537](#) lists the default parameter values of remote Coulomb scattering, which is treated as an intravalley process. These parameters apply to all valleys.

*Table 537 Parameters of remote Coulomb scattering*

Parameter symbol	Parameter name	Mechanism name:	RC	Unit
		Description	Default	
$z_d$	zd	Depth of charge centroid	1.5	nm
$E_0$	E0	Minimum energy for tabulating rate	0	eV
$N_0$	N0	Minimum screening density	$5 \times 10^{15}$	$\text{cm}^{-3}$
$i$	final	Final minimum	Same as initial minimum	—

To define the interface charge density for remote Coulomb scattering, follow the descriptions in [Defining Interface Models on page 217](#). By default, no interface charge is applied.

---

## Valence Band Model

This section describes the valence band model.

---

### Band Edge Parameters

To change the default parameter values of the valence band container model, listed in [Table 538](#), use the following input file syntax:

```
MATERIAL InGaAs.valence.<parameter> <value>
```

*Table 538 Parameters of valence band container model*

Parameter symbol	Parameter name	Description	Interpolation	Unit
$E$	$E$	Valence band energy with respect to vacuum	quadratic	5.26 -0.2 0.43 eV
$m_{dg_x}$	$dgx$	Hole density gradient effective x-mass	constant	0.5 $m_e$
$m_{dg_y}$	$dgy$	Hole density gradient effective y-mass	constant	0.5 $m_e$
$m_{dg_z}$	$dgz$	Hole density gradient effective z-mass	constant	0.5 $m_e$

#### k-p band structure model parameters

$L$	$L-kp$	Valence band parameter	linear	$\hbar^2/2m$
$M$	$M-kp$	Valence band parameter	linear	$\hbar^2/2m$
$N$	$N-kp$	Valence band parameter	linear	$\hbar^2/2m$
$l$	$l-defpot$	Valence deformation potential	linear	eV
$m$	$m-defpot$	Valence deformation potential	linear	eV

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### Valence Band Model

Table 538 Parameters of valence band container model (Continued)

Parameter symbol	Parameter name	Description	Interpolation	Unit
$n$	n-defpot	Valence deformation potential	linear	eV
$\Delta_{\text{SSO}}$	dss0	Spin-orbit split energy	linear	eV

To change the default parameter values of the valence bands in the container model, listed in [Table 539](#), use the following input file syntax:

```
MATERIAL InGaAs.valence.<band>.<parameter> <value>
```

Table 539 Parameters of valence band model

Parameter symbol	Parameter name	Description	Default	Unit
<b>Heavy hole (HH) band</b>				
$E$	E	Valence band energy with respect to container energy	0.0	eV
$model$	model	Model used for transport in this band	6kp	—
<b>Light hole (LH) band</b>				
$E$	E	Valence band energy with respect to container energy	0.0	eV
$model$	model	Model used for transport in this band	6kp	—
<b>Spin split-off (SSO) band</b>				
$E$	E	Valence band energy with respect to container energy	0.044	eV
$model$	model	Model used for transport in this band	6kp	—

## Mobility Models

The valence band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models together with some phenomenological enhancement factors.

## Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 540](#), use the following input file syntax:

```
MATERIAL InGaAs.valence.constant.<parameter> <value>
```

*Table 540 Parameters of constant mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	$\begin{cases} x = 0.0 & 530 \\ x = 0.47 & 320 \\ x = 1.0 & 491.5 \end{cases}$	cm <sup>2</sup> /Vs
$\zeta$	zeta	Fitting parameter	2.2	—

## Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 541](#), use the following input file syntax:

```
MATERIAL InGaAs.valence.Arora.<parameter> <value>
```

*Table 541 Parameters of Arora mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\max}$	mu_max	Maximum mobility	$\begin{cases} x = 0.0 & 530 \\ x = 0.47 & 320 \\ x = 1.0 & 491.5 \end{cases}$	cm <sup>2</sup> /Vs
$\mu_{\min}$	mu_min	Minimum mobility	54.3	cm <sup>2</sup> /Vs
$N_0$	n0	Reference concentration	$2.35 \times 10^{17}$	cm <sup>-3</sup>
$\alpha$	alpha	Fitting parameter	0.88	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.33	—

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 Valence Band Model

*Table 541 Parameters of Arora mobility model (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

## Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 542](#), use the following input file syntax:

```
MATERIAL InGaAs.valence.Masetti.<parameter> <value>
```

*Table 542 Parameters of Masetti mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\max}$	mumax	Maximum mobility	$\begin{cases} x = 0.0 & 530 \\ x = 0.47 & 320 \\ x = 1.0 & 491.5 \end{cases}$	$\text{cm}^2/\text{Vs}$
$\mu_{\min1}$	mumin1	Minimum mobility	75.0	$\text{cm}^2/\text{Vs}$
$\mu_{\min2}$	mumin2	Minimum mobility	75.0	$\text{cm}^2/\text{Vs}$
$\mu_1$	mul1	Maximum mobility	10.0	$\text{cm}^2/\text{Vs}$
$C_r$	cr	Reference concentration	$1.0 \times 10^{18}$	$\text{cm}^{-3}$
$C_s$	cs	Reference solid solubility concentration	1.0	$\text{cm}^{-3}$
$p_c$	pc	Fitting parameter	0.0	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	2.37	—
$\beta$	beta	Fitting parameter	2.0	—
$\zeta$	zeta	Fitting parameter	2.2	—

## Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 543](#), use the following input file syntax:

```
MATERIAL InGaAs.valence.Yamaguchi.<parameter> <value>
```

*Table 543 Parameters of Yamaguchi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

## Perpendicular Field: Lombardi Mobility Model

To change the default parameter values of the Lombardi mobility model, listed in [Table 544](#), use the following input file syntax:

```
MATERIAL InGaAs.valence.Lombardi.<parameter> <value>
```

*Table 544 Parameters of Lombardi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$A$	a	Fitting parameter	2.0	—
$B$	b	Fitting parameter	$9.925 \times 10^6$	cm/s
$C$	c	Fitting parameter	$2.947 \times 10^3$	$\text{cm}^{5/3} \text{V}^{-2/3} \text{s}^{-1}$
$\alpha$	alpha	Fitting parameter	0.0	$\text{cm}^3$
$\delta$	delta	Fitting parameter	$2.0546 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$2.0546 \times 10^{30}$	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	1.0	—
$\lambda$	lambda	Fitting parameter	0.0317	—
$\nu$	nu	Fitting parameter	1.0	—

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**Valence Band Model**

*Table 544 Parameters of Lombardi mobility model (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$N_0$	n0	Fitting parameter	1.0	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	1.0	$\text{cm}^{-3}$
$l_{\text{crit}}$	lcrit	Critical length	$1 \times 10^{-6}$	cm

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in [Table 545](#), use the following input file syntax:

```
MATERIAL InGaAs.valence.Caughey.<parameter> <value>
```

*Table 545 Parameters of Caughey–Thomas mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$4.5 \times 10^6$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	0.52	–
$\beta_0$	beta0	Fitting parameter	1.213	–
$\beta_{\text{exp}}$	bexp	Fitting parameter	0.17	–
$\alpha$	alpha	Fitting parameter	0.0	–

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 546](#). To change the default mobility model, use the following input file syntax:

```
MATERIAL InGaAs.valence.mobility.<model> <value>
```

## Chapter 23: Indium Gallium Arsenide Binary Alloy Material Model

### Valence Band Model

Table 546 Parameters of default mobility model

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley valence band model consists of the valley minima listed in [Table 547](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL InGaAs.valence.<band>.<valley> REMOVE
```

### Note:

The valence band analytic valley approximation is used only as a way to define density-of-states for drift-diffusion simulations and to define the valley minima in response to stress.

Table 547 Names of valence band minima

Valence band minima	Band name	Valley name
Heavy hole	HH	vhh
Light hole	LH	vlh
Spin split-off	SSO	vsso

## Position and Orientation

The position and orientation of the HH, LH, and SSO valley minima are identical. [Table 548](#) shows the default values. To change the default values, use the following input file syntax:

```
MATERIAL InGaAs.valence.<band>.<valley>.min.<parameter> <value>
```

**Chapter 23: Indium Gallium Arsenide Binary Alloy Material Model**  
**Valence Band Model**

*Table 548 Position and orientation parameters of HH, LH, and SSO valley minima*

Parameter symbol	Parameter name	Description	Interpolation	Unit
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$

## Parameters

To change the valley minima model parameters, listed in [Table 549](#), for each valley listed in [Table 547](#), use the following input file syntax:

```
MATERIAL InGaAs.valence.<band>.<valley>.<parameter> <value>
```

*Table 549 Parameters of valence band minima*

Parameter symbol	Parameter name	Description	Interpolation	Unit
<b>Heavy hole (HH) band</b>				
$E$	E	Minima with respect to band edge	linear	eV
$m_x$	mx	Longitudinal effective mass	linear	$m_e$
$m_y$	my	Transverse effective mass	linear	$m_e$
$m_z$	mz	Transverse effective mass	linear	$m_e$
$\alpha$	a	Valley nonparabolicity factor	linear	—
$a_v$	av	Hydrostatic deformation potential	linear	eV
<b>Light hole (LH) band</b>				
$E$	E	Minima with respect to band edge	linear	eV

**Chapter 23: Indium Gallium Arsenide Binary Alloy Material Model**  
**Valence Band Model**

*Table 549 Parameters of valence band minima (Continued)*

Parameter symbol	Parameter name	Description	Interpolation	Unit
$m_x$	mx	Longitudinal effective mass	linear	$m_e$
$m_y$	my	Transverse effective mass	linear	$m_e$
$m_z$	mz	Transverse effective mass	linear	$m_e$
$\alpha$	a	Valley nonparabolicity factor	linear	—
$a_v$	av	Hydrostatic deformation potential	linear	eV
<b>Spin split-off (SSO) band</b>				
$E$	E	Minima with respect to band edge	quadratic	-0.15 eV
$m_x$	mx	Longitudinal effective mass	linear	$m_e$
$m_y$	my	Transverse effective mass	linear	$m_e$
$m_z$	mz	Transverse effective mass	linear	$m_e$
$\alpha$	a	Valley nonparabolicity factor	linear	—
$a_v$	av	Hydrostatic deformation potential	linear	eV

## Heavy-Hole Band Scattering Mechanisms

There are no heavy-hole band scattering mechanisms defined in the current version of Garand.

## Light-Hole Band Scattering Mechanisms

There are no light-hole band scattering mechanisms defined in the current version of Garand.

## **Spin Split-Off Band Scattering Mechanisms**

There are no spin split-off band scattering mechanisms defined in the current version of Garand.

# 24

## Indium Aluminum Arsenide Binary Alloy Material Model

---

*This chapter describes the  $In_{1-x}Al_xAs$  binary alloy material model.*

---

### Bulk Material Model

This section describes the bulk material model for the  $In_{1-x}Al_xAs$  binary alloy material.

---

#### Parameters of Bulk Material Model

To change the default parameter values in [Table 550](#), use the following input file syntax:

```
MATERIAL InAlAs.<parameter> <value>
```

*Table 550 Bulk material model parameters*

Parameter symbol	Parameter name	Description	Interpolation	Default	Unit
<b>Binary material-specific properties</b>					
$x$	x_fraction	Binary alloy fraction	NA	—	—
$A_{1-x}$	material1	Binary alloy constituent material <i>A</i>	NA	InAs	—
$B_x$	material2	Binary alloy constituent material <i>B</i>	NA	AlAs	—
<b>Crystal lattice and orientation in simulation domain</b>					
$ a $	a	Magnitude of lattice vector $a$	linear	—	Å

**Chapter 24: Indium Aluminum Arsenide Binary Alloy Material Model**  
**Bulk Material Model**

*Table 550 Bulk material model parameters (Continued)*

Parameter symbol	Parameter name	Description	Interpolation	Default	Unit
$ b $	b	Magnitude of lattice vector $b$	linear	—	Å
$ c $	c	Magnitude of lattice vector $c$	linear	—	Å
$\alpha$	alpha	Angle between $b$ and $c$	NA	90	degree
$\beta$	beta	Angle between $c$ and $a$	NA	90	degree
$\gamma$	gamma	Angle between $a$ and $b$	NA	90	degree
$\langle hkl \rangle_x$	x	Orientation in the x-direction	NA	1 0 0	—
$\langle hkl \rangle_z$	z	Orientation in the z-direction	NA	0 0 1	—
<b>Bulk electrical and mechanical properties</b>					
$\kappa$	permittivity	Relative dielectric constant	linear	—	—
$\kappa_\infty$	k_inf	High-frequency permittivity	linear	—	—
$\rho$	density	Mass density	linear	—	g/cm <sup>3</sup>
$C_{11}$	c11	Elastic stiffness matrix element	linear	—	GPa
$C_{12}$	c12	Elastic stiffness matrix element	linear	—	GPa
$C_{44}$	c44	Elastic stiffness matrix element	linear	—	GPa

---

## Band-to-Band Tunneling Parameters

To change the default parameter values for the Kane model, listed in [Table 551](#), use the following input file syntax:

```
MATERIAL InAlAs.BTBT.<parameter> <value>
```

*Table 551 Band-to-band tunneling parameters*

Parameter symbol	Parameter name	Description	Default	Unit
$D_{TA}$	DTA	Acoustic phonon deformation potential	0.0	eV
$\epsilon_{TA}$	epsilonTA	Acoustic phonon energy	0.0	eV

---

## Conduction Band Model

This section describes the conduction band model.

---

## Band Edge Parameters

To change the default parameter values of the conduction band container model, listed in [Table 552](#), use the following input file syntax:

```
MATERIAL InAlAs.conduction.<parameter> <value>
```

*Table 552 Parameters of conduction band container model*

Parameter symbol	Parameter name	Description	Interpolation	Default	Unit
$E$	E	Conduction band energy with respect to vacuum	linear	4.2	eV
$m_{dg_x}$	dgx	Electron density gradient effective x-mass	constant	0.3	$m_e$
$m_{dg_y}$	dgy	Electron density gradient effective y-mass	constant	0.3	$m_e$
$m_{dg_z}$	dgz	Electron density gradient effective z-mass	constant	0.3	$m_e$

## Chapter 24: Indium Aluminum Arsenide Binary Alloy Material Model

### Conduction Band Model

To change the default parameter values of the conduction bands in the container model, listed in [Table 553](#), use the following input file syntax:

```
MATERIAL InAlAs.conduction.<band>.<parameter> <value>
```

*Table 553 Parameters of conduction band model*

Parameter symbol	Parameter name	Description	Default	Unit
E	E	Conduction band energy with respect to container energy	0.0	eV
model	model	Model used for transport in this band	ema	—

## Mobility Models

The conduction band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models.

### Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 554](#), use the following input file syntax:

```
MATERIAL InAlAs.conduction.constant.<parameter> <value>
```

*Table 554 Parameters of constant mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	$x = 0.1 \quad 20590$ $x = 0.2 \quad 18580$ $x = 0.3 \quad 16570$ $x = 0.4 \quad 14560$ $x = 0.5 \quad 12550$ $x = 0.6 \quad 10140$ $x = 0.7 \quad 8530$ $x = 0.8 \quad 6520$ $x = 0.9 \quad 4510$	$\text{cm}^2/\text{Vs}$
$\zeta$	zeta	Fitting parameter	2.5	—

## Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 555](#), use the following input file syntax:

```
MATERIAL InAlAs.conduction.Arora.<parameter> <value>
```

*Table 555 Parameters of Arora mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\max}$	mumax	Maximum mobility	$\begin{cases} x = 0.1 & 20590 \\ x = 0.2 & 18580 \\ x = 0.3 & 16570 \\ x = 0.4 & 14560 \\ x = 0.5 & 12550 \\ x = 0.6 & 10140 \\ x = 0.7 & 8530 \\ x = 0.8 & 6520 \\ x = 0.9 & 4510 \end{cases}$	$\text{cm}^2/\text{Vs}$
$\mu_{\min}$	mumin	Minimum mobility	88.0	$\text{cm}^2/\text{Vs}$
$N_0$	n0	Reference concentration	$1.25 \times 10^{17}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.88	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.33	—
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

## Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 556](#), use the following input file syntax:

```
MATERIAL InAlAs.conduction.Masetti.<parameter> <value>
```

**Chapter 24: Indium Aluminum Arsenide Binary Alloy Material Model**  
 Conduction Band Model

*Table 556 Parameters of Masetti mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\max}$	mumax	Maximum mobility	$\begin{cases} x = 0.1 & 20590 \\ x = 0.2 & 18580 \\ x = 0.3 & 16570 \\ x = 0.4 & 14560 \\ x = 0.5 & 12550 \\ x = 0.6 & 10140 \\ x = 0.7 & 8530 \\ x = 0.8 & 6520 \\ x = 0.9 & 4510 \end{cases}$	$\text{cm}^2/\text{Vs}$
$\mu_{\min1}$	mumin1	Minimum mobility	100.0	$\text{cm}^2/\text{Vs}$
$\mu_{\min2}$	mumin2	Minimum mobility	100.0	$\text{cm}^2/\text{Vs}$
$\mu_1$	mul	Maximum mobility	1.0	$\text{cm}^2/\text{Vs}$
$C_r$	cr	Reference concentration	$3.2 \times 10^{17}$	$\text{cm}^{-3}$
$C_s$	cs	Reference solid solubility concentration	0.0	$\text{cm}^{-3}$
$p_c$	pc	Fitting parameter	0.0	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.5	—
$\beta$	beta	Fitting parameter	2.0	—
$\zeta$	zeta	Fitting parameter	2.5	—

## Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 557](#), use the following input file syntax:

```
MATERIAL InAlAs.conduction.Yamaguchi.<parameter> <value>
```

**Chapter 24: Indium Aluminum Arsenide Binary Alloy Material Model**  
 Conduction Band Model

*Table 557 Parameters of Yamaguchi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

## Perpendicular Field: Lombardi Mobility Model

To change the default parameter values of the Lombardi mobility model, listed in [Table 558](#), use the following input file syntax:

```
MATERIAL InAlAs.conduction.Lombardi.<parameter> <value>
```

*Table 558 Parameters of Lombardi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$A$	a	Fitting parameter	2.0	—
$B$	b	Fitting parameter	$4.75 \times 10^7$	cm/s
$C$	c	Fitting parameter	$5.80 \times 10^2$	$\text{cm}^{5/3} \text{V}^{-2/3} \text{s}^{-1}$
$\alpha$	alpha	Fitting parameter	0.0	$\text{cm}^3$
$\delta$	delta	Fitting parameter	$5.82 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$5.82 \times 10^{30}$	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	1.0	—
$\lambda$	lambda	Fitting parameter	0.125	—
$\nu$	nu	Fitting parameter	1.0	—
$N_0$	n0	Fitting parameter	1.0	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	1.0	—
$l_{\text{crit}}$	lcrit	Critical length	$1 \times 10^{-6}$	cm/s

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in [Table 559](#), use the following input file syntax:

```
MATERIAL InAlAs.conduction.Caughey.<parameter> <value>
```

*Table 559 Parameters of Caughey–Thomas mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$1.07 \times 10^7$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	0.87	—
$\beta_0$	beta0	Fitting parameter	1.109	—
$\beta_{\text{exp}}$	bexp	Fitting parameter	0.66	—
$\alpha$	alpha	Fitting parameter	0.0	—

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 560](#). To change the default mobility model, use the following input file syntax:

```
MATERIAL InAlAs.conduction.mobility.<model> <value>
```

*Table 560 Parameters of default mobility model*

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley conduction band model consists of the valley minima listed in [Table 561](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL InAlAs.conduction.<band>.<valley> REMOVE
```

*Table 561 Names of conduction band C1 minima*

Conduction band minimum	Valley name
X	X1, X2, X3, X4, X5, X6
L	L1, L2, L3, L4, L5, L6, L7, L8
$\Gamma$	G

## Position and Orientation

Valley minima differ in their position and orientation, the default values of which are shown in [Table 562](#), [Table 563](#), and [Table 564](#).

To change default values, use the following input file syntax:

```
MATERIAL InAlAs.conduction.C1.<valley>.min.<parameter> <value>
```

*Table 562 Position and orientation parameters of L-minima of conduction band*

Parameter symbol	Parameter name	Description	Interpolation	Unit
<b>L1</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
x	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
y	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
z	z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>L2</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$

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 Conduction Band Model

*Table 562 Position and orientation parameters of L-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Interpolation	Unit
$x$	$x$	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	$y$	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	$z$	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>L3</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	$x$	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	$y$	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	$z$	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>L4</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	$x$	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	$y$	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	$z$	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>L5</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	$x$	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	$y$	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	$z$	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$

**Chapter 24: Indium Aluminum Arsenide Binary Alloy Material Model**  
 Conduction Band Model

*Table 562 Position and orientation parameters of L-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Interpolation	Unit
<b>L6</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>L7</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>L8</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$

**Chapter 24: Indium Aluminum Arsenide Binary Alloy Material Model**  
 Conduction Band Model

*Table 563 Position and orientation parameters of  $\Gamma$ -minimum of conduction band*

Parameter symbol	Parameter name	Description	Interpolation	Unit
<b>G</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$

*Table 564 Position and orientation parameters of X-minima of conduction band*

Parameter symbol	Parameter name	Description	Interpolation	Unit
<b>X1</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>X2</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$

**Chapter 24: Indium Aluminum Arsenide Binary Alloy Material Model**  
 Conduction Band Model

*Table 564 Position and orientation parameters of X-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Interpolation	Unit
<b>X3</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>X4</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>X5</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$
<b>X6</b>				
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$

**Chapter 24: Indium Aluminum Arsenide Binary Alloy Material Model**  
 Conduction Band Model

*Table 564 Position and orientation parameters of X-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Interpolation	Unit
$z$	$z$	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$

## Parameters

To change the default parameter values of the valley minima models, listed in the following tables, for each valley listed in [Table 561](#), use the following input file syntax:

```
MATERIAL InAlAs.conduction.C1.<valley>.<parameter> <value>
```

### Note:

By default, all  $X$ -minima have the same parameter values, and all  $L$ -minima have the same parameter values.

*Table 565 Parameters of L-valley model*

Parameter symbol	Parameter name	Description	Interpolation	Unit
$E$	$E$	Minima with respect to band edge	linear	eV
$m_x$	$mx$	Longitudinal effective mass	linear	$m_e$
$m_y$	$my$	Transverse effective mass	linear	$m_e$
$m_z$	$mz$	Transverse effective mass	linear	$m_e$
$\alpha$	$a$	Valley nonparabolicity factor	linear	—
$\Xi_u$	$xi\_u$	Uniaxial deformation potential	linear	eV
$\Xi_d$	$xi\_d$	Dilatation deformation potential	linear	eV
$\Xi'_u$	$xi\_u\_prime$	Uniaxial mass deformation	linear	eV

**Chapter 24: Indium Aluminum Arsenide Binary Alloy Material Model**  
 Conduction Band Model

*Table 566 Parameters of X-valley model*

Parameter symbol	Parameter name	Description	Interpolation	Unit
$E$	$E$	Minima with respect to band edge	linear	eV
$m_x$	$m_x$	Longitudinal effective mass	linear	$m_e$
$m_y$	$m_y$	Transverse effective mass	linear	$m_e$
$m_z$	$m_z$	Transverse effective mass	linear	$m_e$
$\alpha$	$\alpha$	Valley nonparabolicity factor	linear	—
$\Xi_u$	$\xi_{i\_u}$	Uniaxial deformation potential	linear	eV
$\Xi_d$	$\xi_{i\_d}$	Dilatation deformation potential	linear	eV
$\Xi'_u$	$\xi'_{i\_u\_prime}$	Uniaxial mass deformation	linear	eV

*Table 567 Parameters of  $\Gamma$ -valley model*

Parameter symbol	Parameter name	Description	Interpolation	Unit
$E$	$E$	Minima with respect to band edge	quadraticIII 0.0 0.159 0.7	eV
$m_x$	$m_x$	Longitudinal effective mass	quadraticIII 0.023 0.078 0.049	$m_e$
$m_y$	$m_y$	Transverse effective mass	quadraticIII 0.023 0.078 0.049	$m_e$
$m_z$	$m_z$	Transverse effective mass	quadraticIII 0.023 0.078 0.049	$m_e$
$\alpha$	$\alpha$	Valley nonparabolicity factor	linear	—
$\Xi_u$	$\xi_{i\_u}$	Uniaxial deformation potential	linear	eV

**Chapter 24: Indium Aluminum Arsenide Binary Alloy Material Model**  
 Conduction Band Model

*Table 567 Parameters of  $\Gamma$ -valley model (Continued)*

Parameter symbol	Parameter name	Description	Interpolation	Unit
$\Xi_d$	$\xi_i_d$	Dilatation deformation potential	linear	eV
$\Xi_u$	$\xi_i_u_{\text{prime}}$	Uniaxial mass deformation	linear	eV

## L-Valley Scattering Mechanisms

The eight  $L$ -minima define the set of scattering mechanisms listed in [Table 568](#). By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL InAlAs.conduction.C1.<valley>.<mechanism> ADD
MATERIAL InAlAs.conduction.C1.<valley>.<mechanism> REMOVE
```

*Table 568 Scattering mechanisms for L-minima*

Scattering mechanism	L1	L2	L3	L4	L5	L6	L7	L8
	Mechanism name							
Acoustic Phonon (elastic)	ac	ac	ac	ac	ac	ac	ac	ac
Polar Optical (intra)	pop	pop	pop	pop	pop	pop	pop	pop
Optical Phonon (intra)	opl	opl	opl	opl	opl	opl	opl	opl
Optical Phonon (inter)	opl2	opl1						
Optical Phonon (inter)	opl3	opl3	opl2	opl2	opl2	opl2	opl2	opl2
Optical Phonon (inter)	opl4	opl4	opl4	opl3	opl3	opl3	opl3	opl3
Optical Phonon (inter)	opl5	opl5	opl5	opl5	opl4	opl4	opl4	opl4
Optical Phonon (inter)	opl6	opl6	opl6	opl6	opl6	opl5	opl5	opl5
Optical Phonon (inter)	opl7	opl7	opl7	opl7	opl7	opl7	opl6	opl6

*Table 568 Scattering mechanisms for L-minima (Continued)*

Scattering mechanism	L1	L2	L3	L4	L5	L6	L7	L8
Mechanism name								
Optical Phonon (inter)	opl8	opl7						
Optical Phonon (inter)	opx1							
Optical Phonon (inter)	opx2							
Optical Phonon (inter)	opx3							
Optical Phonon (inter)	opx4							
Optical Phonon (inter)	opx5							
Optical Phonon (inter)	opx6							
Optical Phonon (inter)	opg							
Ionized Impurity	II							
Surface Roughness	SR							
Remote Coulomb	RC							

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each *L*-minimum, listed in [Table 568](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL InAlAs.conduction.C1.<valley>.<mechanism>.<parameter> <value>
```

### Elastic Acoustic Phonon Scattering

[Table 569](#) lists the default parameter values of intravalley elastic acoustic phonon scattering.

*Table 569 Parameters of elastic acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	L[1, 2, 3, 4, 5, 6, 7, 8]	Unit
		Mechanism name:	ac	
		Description	Interpolation	
$\Delta_{\text{ac}}$	D	Acoustic deformation	linear	eV
$v$	v	Velocity	linear	m/s
$i$	final	Final minima	Set from $B_x$ material	–

### Polar-Optical Phonon Scattering

[Table 570](#) lists the default parameter values of intravalley polar-optical phonon scattering.

*Table 570 Parameters of polar-optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L[1, 2, 3, 4, 5, 6, 7, 8]	Unit
		Mechanism name:	pop	
		Description	Interpolation	
$E_{\text{op}}$	E	Phonon energy	linear	eV
$i$	final	Final minima	Set from $B_x$ material	–

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### Optical Phonon Scattering

Table 571 to Table 574 lists the default parameter values of intravalley and intervalley optical phonon scattering.

Table 571 Parameters of intravalley optical phonon scattering

Parameter symbol	Parameter name	Valley name:	L[1, 2, 3, 4, 5, 6, 7, 8]	Unit
		Mechanism name:	opl	
		Description	Interpolation	
$E_{op}$	E	Phonon energy	linear	eV
$D_{op}$	cc	Coupling constant	linear	eV/m
$i$	final	Final minima	Set from $B_x$ material	—

Table 572 Parameters of intervalley L to L optical phonon scattering

Parameter symbol	Parameter name	Valley name:	L[1, 2, 3, 4, 5, 6, 7, 8]	Unit
		Mechanism name:	opl[1, 2, 3, 4, 5, 6, 7, 8]	
		Description	Interpolation	
$E_{op}$	E	Phonon energy	linear	eV
$D_{op}$	cc	Coupling constant	linear	eV/m
$i$	final	Final minima	Set from $B_x$ material	—

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*Table 573 Parameters of intervalley L to  $\Gamma$  optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L[1, 2, 3, 4, 5, 6, 7, 8]	Unit
		Mechanism name:	opg	
		Description	Interpolation	
$E_{\text{op}}$	E	Phonon energy	linear	eV
$D_{\text{op}}$	CC	Coupling constant	linear	eV/m
$i$	final	Final minima	Set from $B_x$ material	—

*Table 574 Parameters of intervalley L to X optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	L[1, 2, 3, 4, 5, 6, 7, 8]	Unit
		Mechanism name:	opx[1, 2, 3, 4, 5, 6]	
		Description	Interpolation	
$E_{\text{op}}$	E	Phonon energy	linear	eV
$D_{\text{op}}$	CC	Coupling constant	linear	eV/m
$i$	final	Final minima	Set from $B_x$ material	—

## $\Gamma$ -Valley Scattering Mechanisms

The  $\Gamma$ -minimum defines the set of scattering mechanisms listed in [Table 575](#). By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL InAlAs.conduction.C2.G.<mechanism> ADD
```

```
MATERIAL InAlAs.conduction.C2.G.<mechanism> REMOVE
```

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*Table 575 Scattering mechanisms for  $\Gamma$ -minimum*

Scattering mechanism	Mechanism name
Acoustic Phonon (elastic)	ac
Polar Optical (intra)	pop
Optical Phonon (inter)	opl1
Optical Phonon (inter)	opl2
Optical Phonon (inter)	opl3
Optical Phonon (inter)	opl4
Optical Phonon (inter)	opl5
Optical Phonon (inter)	opl6
Optical Phonon (inter)	opl7
Optical Phonon (inter)	opl8
Optical Phonon (inter)	opx1
Optical Phonon (inter)	opx2
Optical Phonon (inter)	opx3
Optical Phonon (inter)	opx4
Optical Phonon (inter)	opx5
Optical Phonon (inter)	opx6
Ionized Impurity	II
Surface Roughness	SR
Remote Coulomb	RC

## Parameters of Scattering Mechanisms

To change the default parameter values of the scattering mechanisms listed in [Table 575](#), use the following input file syntax:

```
MATERIAL InAlAs.conduction.C2.G.<mechanism>.<parameter> <value>
```

### Elastic Acoustic Phonon Scattering

[Table 576](#) lists the default parameter values of intravalley elastic acoustic phonon scattering.

*Table 576 Parameters of elastic acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	ac	
		Description	Interpolation	
$\Delta_{ac}$	D	Acoustic deformation	linear	eV
$v$	v	Velocity	linear	m/s
$i$	final	Final minima	Set from $B_x$ material	–

### Polar-Optical Phonon Scattering

[Table 577](#) lists the default parameter values of intravalley polar-optical phonon scattering.

*Table 577 Parameters of polar-optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	pop	
		Description	Interpolation	
$E_{op}$	E	Phonon energy	linear	eV
$i$	final	Final minima	Set from $B_x$ material	–

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### Optical Phonon Scattering

[Table 578](#) and [Table 579](#) list the default parameter values of intervalley optical phonon scattering.

*Table 578 Parameters of intervalley  $\Gamma$  to L optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	opl[1, 2, 3, 4, 5, 6, 7, 8]	
		Description	Interpolation	
$E_{op}$	E	Phonon energy	linear	eV
$D_{op}$	CC	Coupling constant	linear	eV/m
$i$	final	Final minima	Set from $B_x$ material	—

*Table 579 Parameters of intervalley  $\Gamma$  to X optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G	Unit
		Mechanism name:	opx[1, 2, 3, 4, 5, 6]	
		Description	Interpolation	
$E_{op}$	E	Phonon energy	linear	eV
$D_{op}$	CC	Coupling constant	linear	eV/m
$i$	final	Final minima	Set from $B_x$ material	—

---

### X-Valley Scattering Mechanisms

The six X-minima define the set of scattering mechanisms listed in [Table 580](#). By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL InAlAs.conduction.C1.<valley>.<mechanism> ADD
```

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MATERIAL InAlAs.conduction.C1.<valley>.<mechanism> REMOVE

Table 580 Scattering mechanisms for X-minima

Scattering mechanism	X1	X2	X3	X4	X5	X6
	Mechanism name					
Acoustic Phonon (elastic)	ac	ac	ac	ac	ac	ac
Polar Optical (intra)	pop	pop	pop	pop	pop	pop
Optical Phonon (inter)	opx2	opx1	opx1	opx1	opx1	opx1
Optical Phonon (inter)	opx3	opx3	opx2	opx3	opx3	opx3
Optical Phonon (inter)	opx4	opx4	opx4	opx2	opx4	opx4
Optical Phonon (inter)	opx5	opx5	opx5	opx5	opx2	opx5
Optical Phonon (inter)	opx6	opx6	opx6	opx6	opx6	opx2
Optical Phonon (inter)	opl1	opl1	opl1	opl1	opl1	opl1
Optical Phonon (inter)	opl2	opl2	opl2	opl2	opl2	opl2
Optical Phonon (inter)	opl3	opl3	opl3	opl3	opl3	opl3
Optical Phonon (inter)	opl4	opl4	opl4	opl4	opl4	opl4
Optical Phonon (inter)	opl5	opl5	opl5	opl5	opl5	opl5
Optical Phonon (inter)	opl6	opl6	opl6	opl6	opl6	opl6
Optical Phonon (inter)	opl7	opl7	opl7	opl7	opl7	opl7
Optical Phonon (inter)	opl8	opl8	opl8	opl8	opl8	opl8
Optical Phonon (inter)	opg	opg	opg	opg	opg	opg
Ionized Impurity	II	II	II	II	II	II
Surface Roughness	SR	SR	SR	SR	SR	SR
Remote Coulomb	RC	RC	RC	RC	RC	RC

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each  $X$ -minimum, listed in [Table 580](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL InAlAs.conduction.C1.<valley>.<mechanism>.<parameter> <value>
```

### Elastic Acoustic Phonon Scattering

[Table 581](#) lists the default parameter values of intravalley elastic acoustic phonon scattering.

*Table 581 Parameters of elastic acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	X[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	ac	
		Description	Interpolation	
$\Delta_{ac}$	D	Acoustic deformation	linear	eV
$v$	v	Velocity	linear	m/s
$i$	final	Final minima	Set from $B_x$ material	—

### Polar-Optical Phonon Scattering

[Table 582](#) lists the default parameter values of intravalley polar-optical phonon scattering.

*Table 582 Parameters of polar-optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	pop	
		Description	Interpolation	
$E_{op}$	E	Phonon energy	linear	eV
$i$	final	Final minima	Set from $B_x$ material	—

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### Optical Phonon Scattering

Table 583 to Table 585 list the default parameter values of intervalley optical phonon scattering.

Table 583 Parameters of intervalley X to X optical phonon scattering

Parameter symbol	Parameter name	Valley name:	X[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	opx[1, 2, 3, 4, 5, 6]	
		Description	Interpolation	
$E_{\text{op}}$	E	Phonon energy	linear	eV
$D_{\text{op}}$	cc	Coupling constant	linear	eV/m
$i$	final	Final minima	Set from $B_x$ material	—

Table 584 Parameters of intervalley X to L optical phonon scattering

Parameter symbol	Parameter name	Valley name:	X[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	opl[1, 2, 3, 4, 5, 6, 7, 8]	
		Description	Interpolation	
$E_{\text{op}}$	E	Phonon energy	linear	eV
$D_{\text{op}}$	cc	Coupling constant	linear	eV/m
$i$	final	Final minima	Set from $B_x$ material	—

*Table 585 Parameters of intervalley X to  $\Gamma$  optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	X[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	opg	
		Description	Interpolation	
$E_{\text{op}}$	E	Phonon energy	linear	eV
$D_{\text{op}}$	cc	Coupling constant	linear	eV/m
$i$	final	Final minima	Set from $B_x$ material	—

## Ionized Impurity Scattering

Ionized impurity scattering is defined for each valley in a conduction band and is treated as an intravalley process by default, so that the final valley after scattering is the same as the initial valley.

*Table 586 Parameters of ionized impurity scattering*

Parameter symbol	Parameter name	Valley name:	All valleys	Unit
		Mechanism name:	II	
		Description	Default	
$i$	final	Final minimum	Same as initial minimum	—

## Ionized Impurity Empirical Rate Factor

The ionized impurity scattering model includes a scaling factor for the empirical correction of the calculated scattering rate as a function of doping density.

To redefine the default empirical factor, use the following input file syntax:

```
MATERIAL InAlAs.conduction.IIfac N <Nvalue> [<Nvalue2>] <rule> <value>
```

Here, **IIfac** is a piecewise interpolation parameter that defines a correction factor **<value>** for a value **<Nvalue>** of the doping concentration **N**. The interpolation model used to return values between specified densities is given by **<rule>**, which might require an upper bound

of the density [ $<\text{Nvalue2}>$ ]. For a description of the interpolation parameter type, see [Interpolation Methods on page 301](#).

By default, the empirical correction for ionized impurity is 1.0. However, for holes in the material, a non-unity default value is provided to best match experimental low-field concentration-dependent mobility.

## Surface Roughness Scattering

[Table 587](#) lists the default parameter values of surface roughness scattering. These parameters apply to all valleys and to all equivalent surface orientations.

*Table 587 Parameters of surface roughness scattering*

Parameter symbol	Parameter name	Mechanism name:	SR		Unit
		Description	Default		
$\Delta$	rms	RMS amplitude	0.70	0.10	nm
$L_c$	l	Correlation length	2.00	0.30	nm
$\langle hkl \rangle$	orient	Surface orientation	(001)	(110)	–
$i$	carrier	Carrier type	holes	holes	–

## Remote Coulomb Scattering

[Table 588](#) lists the default parameter values of remote Coulomb scattering, which is treated as an intravalley process. These parameters apply to all valleys.

*Table 588 Parameters of remote Coulomb scattering*

Parameter symbol	Parameter name	Mechanism name:	RC		Unit
		Description	Default		
$z_d$	zd	Depth of charge centroid	1.5		nm
$E_0$	E0	Minimum energy for tabulating rate	0		eV
$N_0$	N0	Minimum screening density	$5 \times 10^{15}$		$\text{cm}^{-3}$

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### Valence Band Model

*Table 588 Parameters of remote Coulomb scattering (Continued)*

Parameter symbol	Parameter name	Mechanism name:	RC	Unit
		Description		
<i>i</i>	f <sub>final</sub>	Final minimum	Same as initial minimum	–

To define the interface charge density for remote Coulomb scattering, follow the descriptions in [Defining Interface Models on page 217](#). By default, no interface charge is applied.

## Valence Band Model

This section describes the valence band model.

### Band Edge Parameters

To change the default parameter values of the valence band container model, listed in [Table 589](#), use the following input file syntax:

```
MATERIAL InAlAs.valence.<parameter> <value>
```

*Table 589 Parameters of valence band container model*

Parameter symbol	Parameter name	Description	Interpolation	Unit
<i>E</i>	E	Valence band energy with respect to vacuum	linear	eV
<i>m<sub>dg</sub><sub>x</sub></i>	dgx	Hole density gradient effective x-mass	constant 0.5	<i>m<sub>e</sub></i>
<i>m<sub>dg</sub><sub>y</sub></i>	dgy	Hole density gradient effective y-mass	constant 0.5	<i>m<sub>e</sub></i>
<i>m<sub>dg</sub><sub>z</sub></i>	dgz	Hole density gradient effective z-mass	constant 0.5	<i>m<sub>e</sub></i>
<b>k-p band structure model parameters</b>				
<i>L</i>	L-kp	Valence band parameter	linear	$\hbar^2/2m$
<i>M</i>	M-kp	Valence band parameter	linear	$\hbar^2/2m$

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### Valence Band Model

Table 589 Parameters of valence band container model (Continued)

Parameter symbol	Parameter name	Description	Interpolation	Unit
$N$	N-kp	Valence band parameter	linear	$\hbar^2/2m$
$l$	l-defpot	Valence deformation potential	linear	eV
$m$	m-defpot	Valence deformation potential	linear	eV
$n$	n-defpot	Valence deformation potential	linear	eV
$\Delta_{\text{ss}}\text{o}$	dsso	Spin-orbit split energy	linear	eV

To change the default parameter values of the valence bands in the container model, listed in [Table 590](#), use the following input file syntax:

```
MATERIAL InAlAs.valence.<band>.<parameter> <value>
```

Table 590 Parameters of valence band model

Parameter symbol	Parameter name	Description	Default	Unit
<b>Heavy hole (HH) band</b>				
$E$	E	Valence band energy with respect to container energy	0.0	eV
$model$	model	Model used for transport in this band	6kp	—
<b>Light hole (LH) band</b>				
$E$	E	Valence band energy with respect to container energy	0.0	eV
$model$	model	Model used for transport in this band	6kp	—
<b>Spin split-off (SSO) band</b>				
$E$	E	Valence band energy with respect to container energy	0.044	eV
$model$	model	Model used for transport in this band	6kp	—

---

## Mobility Models

The valence band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models together with some phenomenological enhancement factors.

### Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 591](#), use the following input file syntax:

```
MATERIAL InAlAs.valence.constant.<parameter> <value>
```

*Table 591 Parameters of constant mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	$\begin{cases} x = 0.1 & 240 \\ x = 0.2 & 230 \\ x = 0.3 & 220 \\ x = 0.4 & 210 \\ x = 0.5 & 200 \\ x = 0.6 & 190 \\ x = 0.7 & 180 \\ x = 0.8 & 170 \\ x = 0.9 & 160 \end{cases}$	$\text{cm}^2/\text{Vs}$
$\zeta$	zeta	Fitting parameter	2.2	—

### Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 592](#), use the following input file syntax:

```
MATERIAL InAlAs.valence.Arora.<parameter> <value>
```

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 Valence Band Model

*Table 592 Parameters of Arora mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\max}$	mumax	Maximum mobility	$\begin{cases} x = 0.1 & 240 \\ x = 0.2 & 230 \\ x = 0.3 & 220 \\ x = 0.4 & 210 \\ x = 0.5 & 200 \\ x = 0.6 & 190 \\ x = 0.7 & 180 \\ x = 0.8 & 170 \\ x = 0.9 & 160 \end{cases}$	$\text{cm}^2/\text{Vs}$
$\mu_{\min}$	mumin	Minimum mobility	54.3	$\text{cm}^2/\text{Vs}$
$N_0$	n0	Reference concentration	$2.35 \times 10^{17}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.88	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.33	—
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

### Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 593](#), use the following input file syntax:

```
MATERIAL InAlAs.valence.Masetti.<parameter> <value>
```

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*Table 593 Parameters of Masetti mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\max}$	mumax	Maximum mobility	$\begin{cases} x = 0.1 & 240 \\ x = 0.2 & 230 \\ x = 0.3 & 220 \\ x = 0.4 & 210 \\ x = 0.5 & 200 \\ x = 0.6 & 190 \\ x = 0.7 & 180 \\ x = 0.8 & 170 \\ x = 0.9 & 160 \end{cases}$	$\text{cm}^2/\text{Vs}$
$\mu_{\min1}$	mumin1	Minimum mobility	44.9	$\text{cm}^2/\text{Vs}$
$\mu_{\min2}$	mumin2	Minimum mobility	0.0	$\text{cm}^2/\text{Vs}$
$\mu_1$	mul	Maximum mobility	29.0	$\text{cm}^2/\text{Vs}$
$C_r$	cr	Reference concentration	$1.0 \times 10^{17}$	$\text{cm}^{-3}$
$C_s$	cs	Reference solid solubility concentration	$6.1 \times 10^{20}$	$\text{cm}^{-3}$
$p_c$	pc	Fitting parameter	$9.23 \times 10^{16}$	$\text{cm}^{-3}$
$\alpha$	alpha	Fitting parameter	0.719	—
$\beta$	beta	Fitting parameter	2.0	—
$\zeta$	zeta	Fitting parameter	2.2	—

## Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 594](#), use the following input file syntax:

```
MATERIAL InAlAs.valence.Yamaguchi.<parameter> <value>
```

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 Valence Band Model

*Table 594 Parameters of Yamaguchi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

## Perpendicular Field: Lombardi Mobility Model

To change the default parameter values of the Lombardi mobility model, listed in [Table 595](#), use the following input file syntax:

```
MATERIAL InAlAs.valence.Lombardi.<parameter> <value>
```

*Table 595 Parameters of Lombardi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$A$	a	Fitting parameter	2.0	—
$B$	b	Fitting parameter	$9.925 \times 10^6$	cm/s
$C$	c	Fitting parameter	$2.947 \times 10^3$	$\text{cm}^{5/3} \text{V}^{-2/3} \text{s}^{-1}$
$\alpha$	alpha	Fitting parameter	0.0	$\text{cm}^3$
$\delta$	delta	Fitting parameter	$2.0546 \times 10^{14}$	$\text{cm}^2/\text{Vs}$
$\eta$	eta	Fitting parameter	$2.0546 \times 10^{30}$	$\text{V}^2/\text{cms}$
$\kappa$	k	Fitting parameter	1.0	—
$\lambda$	lambda	Fitting parameter	0.0317	—
$\nu$	nu	Fitting parameter	1.0	—
$N_0$	n0	Fitting parameter	1.0	$\text{cm}^{-3}$
$N_1$	n1	Fitting parameter	1.0	$\text{cm}^{-3}$
$l_{\text{crit}}$	lcrit	Critical length	$1 \times 10^{-6}$	cm

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in [Table 596](#), use the following input file syntax:

```
MATERIAL InAlAs.valence.Caughey.<parameter> <value>
```

*Table 596 Parameters of Caughey–Thomas mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$8.37 \times 10^6$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	0.52	–
$\beta_0$	beta0	Fitting parameter	1.213	–
$\beta_{\text{exp}}$	bexp	Fitting parameter	0.17	–
$\alpha$	alpha	Fitting parameter	0.0	–

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 597](#). To change the default mobility model, use the following input file syntax:

```
MATERIAL InAlAs.valence.mobility.<model> <value>
```

*Table 597 Parameters of default mobility model*

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley valence band model consists of the valley minima listed in [Table 598](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL InAlAs.valence.<band>.<valley> REMOVE
```

**Note:**

The valence band analytic valley approximation is used only as a way to define density-of-states for drift-diffusion simulations and to define the valley minima in response to stress.

*Table 598 Names of valence band minima*

Valence band minima	Band name	Valley name
Heavy hole	HH	vhh
Light hole	LH	vlh
Spin split-off	SSO	vsso

## Position and Orientation

The position and orientation of the HH, LH, and SSO valley minima are identical. [Table 599](#) shows the default values. To change the default values, use the following input file syntax:

```
MATERIAL InAlAs.valence.<band>.<valley>.min.<parameter> <value>
```

*Table 599 Position and orientation parameters of HH, LH, and SSO valley minima*

Parameter symbol	Parameter name	Description	Interpolation	Unit
$k_0$	pos	Position within the Brillouin zone	Set from $B_x$ material	$2\pi/a$
$x$	x	Orientation of the x-axis	Set from $B_x$ material	$\langle hkl \rangle$
$y$	y	Orientation of the y-axis	Set from $B_x$ material	$\langle hkl \rangle$
$z$	z	Orientation of the z-axis	Set from $B_x$ material	$\langle hkl \rangle$

## Parameters

To change the valley minima model parameters, listed in [Table 600](#), for each valley listed in [Table 598](#), use the following input file syntax:

```
MATERIAL InAlAs.valence.<band>.<valley>.<parameter> <value>
```

*Table 600 Parameters of valence band minima*

Parameter symbol	Parameter name	Description	Interpolation	Unit
<b>Heavy hole (HH) band</b>				
$E$	E	Minima with respect to band edge	linear	eV
$m_x$	mx	Longitudinal effective mass	linear	$m_e$
$m_y$	my	Transverse effective mass	linear	$m_e$
$m_z$	mz	Transverse effective mass	linear	$m_e$
$\alpha$	a	Valley nonparabolicity factor	linear	—
$a_v$	av	Hydrostatic deformation potential	linear	eV
<b>Light hole (LH) band</b>				
$E$	E	Minima with respect to band edge	linear	eV
$m_x$	mx	Longitudinal effective mass	linear	$m_e$
$m_y$	my	Transverse effective mass	linear	$m_e$
$m_z$	mz	Transverse effective mass	linear	$m_e$
$\alpha$	a	Valley nonparabolicity factor	linear	—
$a_v$	av	Hydrostatic deformation potential	linear	eV

**Chapter 24: Indium Aluminum Arsenide Binary Alloy Material Model**  
 Valence Band Model

*Table 600 Parameters of valence band minima (Continued)*

Parameter symbol	Parameter name	Description	Interpolation	Unit
<b>Spin split-off (SSO) band</b>				
$E$	$E$	Minima with respect to band edge	quadratic	0.39 –0.24 0.15 eV
$m_x$	$m_x$	Longitudinal effective mass	linear	$m_e$
$m_y$	$m_y$	Transverse effective mass	linear	$m_e$
$m_z$	$m_z$	Transverse effective mass	linear	$m_e$
$\alpha$	$a$	Valley nonparabolicity factor	linear	–
$a_v$	$a_v$	Hydrostatic deformation potential	linear	eV

---

## Heavy-Hole Band Scattering Mechanisms

There are no heavy-hole band scattering mechanisms defined in the current version of Garand.

---

## Light-Hole Band Scattering Mechanisms

There are no light-hole band scattering mechanisms defined in the current version of Garand.

---

## Spin Split-Off Band Scattering Mechanisms

There are no spin split-off band scattering mechanisms defined in the current version of Garand.

# 25

## Gallium Nitride Material Model

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*This chapter describes the GaN material model.*

---

### Bulk Material Model

This section describes the bulk material model for GaN.

---

#### Parameters of Bulk Material Model

To change the default parameter values in [Table 601](#), use the following input file syntax:

```
MATERIAL GaN.<parameter> <value>
```

*Table 601 Bulk material model parameters*

Parameter symbol	Parameter name	Description	Default	Unit
<b>Crystal lattice and orientation in simulation domain</b>				
a	a	Magnitude of lattice vector a	3.189	Å
b	b	Magnitude of lattice vector b	3.189	Å
c	c	Magnitude of lattice vector c	5.185	Å
$\alpha$	alpha	Angle between b and c	90	degree
$\beta$	beta	Angle between c and a	90	degree
$\gamma$	gamma	Angle between a and b	120	degree
$\langle hkl \rangle_x$	x	Orientation in the x-direction	1 0 0	—

## Chapter 25: Gallium Nitride Material Model

### Bulk Material Model

*Table 601 Bulk material model parameters (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
$\langle hkl \rangle_z$	z	Orientation in the z-direction	0 0 1	—
<b>Bulk electrical and mechanical properties</b>				
$\kappa$	permittivity	Relative dielectric constant	8.90	—
$\kappa_\infty$	k_inf	High-frequency permittivity	5.35	—
$\rho$	density	Mass density	6.15	g/cm <sup>3</sup>
$C_{11}$	c11	Elastic stiffness matrix element	390	GPa
$C_{12}$	c12	Elastic stiffness matrix element	145	GPa
$C_{44}$	c44	Elastic stiffness matrix element	105	GPa

## Band-to-Band Tunneling Parameters

To change the default parameter values for the Kane model, listed in [Table 602](#), use the following input file syntax:

```
MATERIAL GaN.BTBT.<parameter> <value>
```

*Table 602 Band-to-band tunneling parameters*

Parameter symbol	Parameter name	Description	Default	Unit
$D_{TA}$	DTA	Acoustic phonon deformation potential	0.0	eV
$\epsilon_{TA}$	epsilonTA	Acoustic phonon energy	0.0	eV

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

---

## Conduction Band Model

This section describes the conduction band model.

---

### Band Edge Parameters

To change the default parameter values of the conduction band container model, listed in [Table 603](#), use the following input file syntax:

```
MATERIAL GaN.conduction.<parameter> <value>
```

*Table 603 Parameters of conduction band container model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Conduction band energy with respect to vacuum	3.95856	eV
$m_{dg_x}$	$dgx$	Electron density gradient effective x-mass	0.5	$m_e$
$m_{dg_y}$	$dgy$	Electron density gradient effective y-mass	0.5	$m_e$
$m_{dg_z}$	$dgz$	Electron density gradient effective z-mass	0.5	$m_e$

To change the default parameter values of the conduction bands in the container model, listed in [Table 604](#), use the following input file syntax:

```
MATERIAL GaN.conduction.<band>.<parameter> <value>
```

*Table 604 Parameters of conduction band model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	$E$	Conduction band energy with respect to container energy	0.0	eV
$model$	$model$	Model used for transport in this band	ema	—

---

## Mobility Models

The conduction band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models.

### Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 605](#), use the following input file syntax:

```
MATERIAL GaN.conduction.constant.<parameter> <value>
```

*Table 605 Parameters of constant mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	1500	cm <sup>2</sup> /Vs
$\zeta$	zeta	Fitting parameter	1	—

### Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 606](#), use the following input file syntax:

```
MATERIAL GaN.conduction.Arora.<parameter> <value>
```

*Table 606 Parameters of Arora mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min}$	mumin	Minimum mobility	160	cm <sup>2</sup> /Vs
$\mu_{\max}$	mumax	Maximum mobility	1460	cm <sup>2</sup> /Vs
$N_0$	n0	Reference concentration	$3 \times 10^{17}$	cm <sup>-3</sup>
$\alpha$	alpha	Fitting parameter	0.66	—
$\beta_1$	b1	Fitting parameter	-1.02	—
$\beta_2$	b2	Fitting parameter	-3.84	—
$\beta_3$	b3	Fitting parameter	3.02	—

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

Table 606 Parameters of Arora mobility model (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$\beta_4$	b4	Fitting parameter	0.81	—

## Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 607](#), use the following input file syntax:

```
MATERIAL GaN.conduction.Masetti.<parameter> <value>
```

Table 607 Parameters of Masetti mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min 1}$	mumin1	Minimum mobility	175	cm <sup>2</sup> /Vs
$\mu_{\min 2}$	mumin2	Minimum mobility	75	cm <sup>2</sup> /Vs
$\mu_{\max}$	mumax	Maximum mobility	1500	cm <sup>2</sup> /Vs
$\mu_1$	mul	Maximum mobility	20	cm <sup>2</sup> /Vs
$C_r$	cr	Reference concentration	$6.5 \times 10^{15}$	cm <sup>-3</sup>
$C_s$	cs	Reference solid solubility concentration	$9.5 \times 10^{16}$	cm <sup>-3</sup>
$p_c$	pc	Reference concentration	$1 \times 10^{16}$	cm <sup>-3</sup>
$\alpha$	alpha	Fitting parameter	0.55	—
$\beta$	beta	Fitting parameter	0.75	—
$\zeta$	zeta	Fitting parameter	1.0	—

## Chapter 25: Gallium Nitride Material Model

Conduction Band Model

### Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 608](#), use the following input file syntax:

```
MATERIAL GaN.conduction.Yamaguchi.<parameter> <value>
```

*Table 608 Parameters of Yamaguchi mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

### High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in [Table 609](#), use the following input file syntax:

```
MATERIAL GaN.conduction.Caughey.<parameter> <value>
```

*Table 609 Parameters of Caughey–Thomas mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$v_{sat}$	vsat	Saturation velocity	$1.8 \times 10^7$	cm/s
$v_{exp}$	vexp	Fitting parameter	1.7	—
$\beta_0$	beta0	Fitting parameter	1	—
$\beta_{exp}$	bexp	Fitting parameter	1	—
$\alpha$	alpha	Fitting parameter	0	—

### Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 610](#). To change the default mobility model, use the following input file syntax:

```
MATERIAL GaN.conduction.mobility.<model> <value>
```

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

Table 610 Parameters of default mobility model

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field-dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley conduction band model consists of the valley minima listed in [Table 611](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL GaN.conduction.<band>.<valley> REMOVE
```

Table 611 Names of conduction band C1 minima

Conduction band minimum	Valley name
C1	
G1	G1
U	U1, U2, U3, U4, U5, U6, U7, U8, U9, U10, U11, U12
M	M1, M2, M3, M4, M5, M6
K	K1, K2, K3, K4, K5, K6
C2	
G3	G3

## Position and Orientation

Valley minima differ in their position and orientation, the default values of which are shown in [Table 612](#) to [Table 616](#).

The G1-valleys and all of the U-valleys, M-valleys, and K-valleys sit in the first conduction band, C1, and are referenced as:

```
MATERIAL GaN.conduction.C1.<valley>.min.<parameter> <value>
```

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

The G3-valley, however, sits in the second conduction band, C2, and is referenced as:

```
MATERIAL GaN.conduction.C2.<valley>.min.<parameter> <value>
```

*Table 612 Position and orientation parameters of G1-minimum of conduction band*

Parameter symbol	Parameter name	Description	Default	Unit
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.0	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	X	Orientation of the x-axis	0 0 0 1	$\langle hki \rangle$
y	Y	Orientation of the y-axis	2 -1 -1 0	$\langle hki \rangle$
z	Z	Orientation of the z-axis	0 1 -1 0	$\langle hki \rangle$

*Table 613 Position and orientation parameters of G3-minimum of conduction band*

Parameter symbol	Parameter name	Description	Default	Unit
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.0	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	X	Orientation of the x-axis	0 0 0 1	$\langle hki \rangle$
y	Y	Orientation of the y-axis	2 -1 -1 0	$\langle hki \rangle$
z	Z	Orientation of the z-axis	0 1 -1 0	$\langle hki \rangle$

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

Table 614 Position and orientation parameters of U-minima of conduction band

Parameter symbol	Parameter name	Description	Default	Unit
<b>U1</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 0.75 0.375	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	x	Orientation of the x-axis	0 1 -1 0	$\langle h k i l \rangle$
y	y	Orientation of the y-axis	-2 1 1 0	$\langle h k i l \rangle$
z	z	Orientation of the z-axis	0 0 0 1	$\langle h k i l \rangle$
<b>U2</b>				
$k_0$	pos	Position within the Brillouin zone	1.0 0.0 0.375	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	x	Orientation of the x-axis	1 0 -1 0	$\langle h k i l \rangle$
y	y	Orientation of the y-axis	-1 2 -1 0	$\langle h k i l \rangle$
z	z	Orientation of the z-axis	0 0 0 1	$\langle h k i l \rangle$
<b>U3</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 -0.75 0.375	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	x	Orientation of the x-axis	1 -1 0 0	$\langle h k i l \rangle$
y	y	Orientation of the y-axis	1 1 -2 0	$\langle h k i l \rangle$
z	z	Orientation of the z-axis	0 0 0 1	$\langle h k i l \rangle$
<b>U4</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 -0.75 0.375	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

*Table 614 Position and orientation parameters of U-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
x	X	Orientation of the x-axis	0 -1 1 0	$\langle\text{hkil}\rangle$
y	Y	Orientation of the y-axis	2 -1 -1 0	$\langle\text{hkil}\rangle$
z	Z	Orientation of the z-axis	0 0 0 1	$\langle\text{hkil}\rangle$
<b>U5</b>				
$k_0$	pos	Position within the Brillouin zone	-1.0 0.0 0.375	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	X	Orientation of the x-axis	-1 0 1 0	$\langle\text{hkil}\rangle$
y	Y	Orientation of the y-axis	1 -2 1 0	$\langle\text{hkil}\rangle$
z	Z	Orientation of the z-axis	0 0 0 1	$\langle\text{hkil}\rangle$
<b>U6</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 0.75 0.375	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	X	Orientation of the x-axis	-1 1 0 0	$\langle\text{hkil}\rangle$
y	Y	Orientation of the y-axis	-1 -1 2 0	$\langle\text{hkil}\rangle$
z	Z	Orientation of the z-axis	0 0 0 1	$\langle\text{hkil}\rangle$
<b>U7</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 0.75 -0.375	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	X	Orientation of the x-axis	0 1 -1 0	$\langle\text{hkil}\rangle$
y	Y	Orientation of the y-axis	-2 1 1 0	$\langle\text{hkil}\rangle$
z	Z	Orientation of the z-axis	0 0 0 1	$\langle\text{hkil}\rangle$

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

*Table 614 Position and orientation parameters of U-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
<b>U8</b>				
$k_0$	pos	Position within the Brillouin zone	1.0 0.0 -0.375	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	x	Orientation of the x-axis	1 0 -1 0	$\langle h k i l \rangle$
y	y	Orientation of the y-axis	-1 2 -1 0	$\langle h k i l \rangle$
z	z	Orientation of the z-axis	0 0 0 1	$\langle h k i l \rangle$
<b>U9</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 -0.75 -0.375	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	x	Orientation of the x-axis	1 -1 0 0	$\langle h k i l \rangle$
y	y	Orientation of the y-axis	1 1 -2 0	$\langle h k i l \rangle$
z	z	Orientation of the z-axis	0 0 0 1	$\langle h k i l \rangle$
<b>U10</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 -0.75 -0.375	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	x	Orientation of the x-axis	0 -1 1 0	$\langle h k i l \rangle$
y	y	Orientation of the y-axis	2 -1 -1 0	$\langle h k i l \rangle$
z	z	Orientation of the z-axis	0 0 0 1	$\langle h k i l \rangle$
<b>U11</b>				
$k_0$	pos	Position within the Brillouin zone	-1.0 0.0 -0.375	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

*Table 614 Position and orientation parameters of U-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
x	x	Orientation of the x-axis	-1 0 1 0	$\langle \text{hkil} \rangle$
y	y	Orientation of the y-axis	1 -2 1 0	$\langle \text{hkil} \rangle$
z	z	Orientation of the z-axis	0 0 0 1	$\langle \text{hkil} \rangle$
<b>U12</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 0.75 -0.375	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	x	Orientation of the x-axis	-1 1 0 0	$\langle \text{hkil} \rangle$
y	y	Orientation of the y-axis	-1 -1 2 0	$\langle \text{hkil} \rangle$
z	z	Orientation of the z-axis	0 0 0 1	$\langle \text{hkil} \rangle$

*Table 615 Position and orientation parameters of M-minima of conduction band*

Parameter symbol	Parameter name	Description	Default	Unit
<b>M1</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 0.75 0.0	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	x	Orientation of the x-axis	0 1 -1 0	$\langle \text{hkil} \rangle$
y	y	Orientation of the y-axis	-2 1 1 0	$\langle \text{hkil} \rangle$
z	z	Orientation of the z-axis	0 0 0 1	$\langle \text{hkil} \rangle$

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

Table 615 Position and orientation parameters of M-minima of conduction band (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
<b>M2</b>				
$k_0$	pos	Position within the Brillouin zone	1.0 0.0 0.0	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	x	Orientation of the x-axis	1 0 -1 0	$\langle h k i l \rangle$
y	y	Orientation of the y-axis	-1 2 -1 0	$\langle h k i l \rangle$
z	z	Orientation of the z-axis	0 0 0 1	$\langle h k i l \rangle$
<b>M3</b>				
$k_0$	pos	Position within the Brillouin zone	0.5 -0.75 0.0	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	x	Orientation of the x-axis	1 -1 0 0	$\langle h k i l \rangle$
y	y	Orientation of the y-axis	1 1 -2 0	$\langle h k i l \rangle$
z	z	Orientation of the z-axis	0 0 0 1	$\langle h k i l \rangle$
<b>M4</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 -0.75 0.0	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	x	Orientation of the x-axis	0 -1 1 0	$\langle h k i l \rangle$
y	y	Orientation of the y-axis	2 -1 -1 0	$\langle h k i l \rangle$
z	z	Orientation of the z-axis	0 0 0 1	$\langle h k i l \rangle$
<b>M5</b>				
$k_0$	pos	Position within the Brillouin zone	-1.0 0.0 0.0	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

*Table 615 Position and orientation parameters of M-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
x	x	Orientation of the x-axis	-1 0 1 0	$\langle\text{hkil}\rangle$
y	y	Orientation of the y-axis	1 -2 1 0	$\langle\text{hkil}\rangle$
z	z	Orientation of the z-axis	0 0 0 1	$\langle\text{hkil}\rangle$
<b>M6</b>				
$k_0$	pos	Position within the Brillouin zone	-0.5 0.75 0.0	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	x	Orientation of the x-axis	-1 1 0 0	$\langle\text{hkil}\rangle$
y	y	Orientation of the y-axis	-1 -1 2 0	$\langle\text{hkil}\rangle$
z	z	Orientation of the z-axis	0 0 0 1	$\langle\text{hkil}\rangle$

*Table 616 Position and orientation parameters of K-minima of conduction band*

Parameter symbol	Parameter name	Description	Default	Unit
<b>K1</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 1.0 0.0	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	x	Orientation of the x-axis	-1 2 -1 0	$\langle\text{hkil}\rangle$
y	y	Orientation of the y-axis	-1 0 1 0	$\langle\text{hkil}\rangle$
z	z	Orientation of the z-axis	0 0 0 1	$\langle\text{hkil}\rangle$

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

*Table 616 Position and orientation parameters of K-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
<b>K2</b>				
$k_0$	pos	Position within the Brillouin zone	1.0 0.5 0.0	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	x	Orientation of the x-axis	1 1 -2 0	$\langle h k i l \rangle$
y	y	Orientation of the y-axis	-1 1 0 0	$\langle h k i l \rangle$
z	z	Orientation of the z-axis	0 0 0 1	$\langle h k i l \rangle$
<b>K3</b>				
$k_0$	pos	Position within the Brillouin zone	1.0 -0.5 0.0	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	x	Orientation of the x-axis	2 -1 -1 0	$\langle h k i l \rangle$
y	y	Orientation of the y-axis	0 1 -1 0	$\langle h k i l \rangle$
z	z	Orientation of the z-axis	0 0 0 1	$\langle h k i l \rangle$
<b>K4</b>				
$k_0$	pos	Position within the Brillouin zone	0.0 -1.0 0.0	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	x	Orientation of the x-axis	1 -2 1 0	$\langle h k i l \rangle$
y	y	Orientation of the y-axis	1 0 -1 0	$\langle h k i l \rangle$
z	z	Orientation of the z-axis	0 0 0 1	$\langle h k i l \rangle$
<b>K5</b>				
$k_0$	pos	Position within the Brillouin zone	-1.0 -0.5 0.0	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

*Table 616 Position and orientation parameters of K-minima of conduction band (Continued)*

Parameter symbol	Parameter name	Description	Default	Unit
x	x	Orientation of the x-axis	-1 -1 2 0	$\langle \text{hkil} \rangle$
y	y	Orientation of the y-axis	1 -1 0 0	$\langle \text{hkil} \rangle$
z	z	Orientation of the z-axis	0 0 0 1	$\langle \text{hkil} \rangle$
<b>K6</b>				
$k_0$	pos	Position within the Brillouin zone	-1.0 0.5 0.0	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
x	x	Orientation of the x-axis	-2 1 1 0	$\langle \text{hkil} \rangle$
y	y	Orientation of the y-axis	0 -1 1 0	$\langle \text{hkil} \rangle$
z	z	Orientation of the z-axis	0 0 0 1	$\langle \text{hkil} \rangle$

## Parameters

To change the default parameter values of the valley minima models, listed in the following tables, for each valley listed in [Table 611](#), use the following input file syntax:

```
MATERIAL GaN.conduction.<band>.<valley>.<parameter> <value>
```

### Note:

By default, all M-minima have the same parameter values, all U-minima have the same parameter values, and all K-minima have the same parameter values.

*Table 617 Parameters of G1-valley model*

Parameter symbol	Parameter name	Description	Default	Unit
E	E	Minima with respect to band edge	0.0	eV
$m_x$	mx	Longitudinal effective mass	0.21	$m_e$
$m_y$	my	Transverse effective mass	0.2	$m_e$

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Table 617 Parameters of G1-valley model (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$m_z$	mz	Transverse effective mass	0.2	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.189	—
$Z_f$	zf	Fraction of the valley within the first Brillouin zone	1.0	—

Table 618 Parameters of G3-valley model

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Minima with respect to band edge	1.9	eV
$m_x$	mx	Longitudinal effective mass	0.6	$m_e$
$m_y$	my	Transverse effective mass	0.6	$m_e$
$m_z$	mz	Transverse effective mass	0.6	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.029	—
$Z_f$	zf	Fraction of the valley within the first Brillouin zone	1.0	—

Table 619 Parameters of U-valley model

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Minima with respect to band edge	2.1	eV
$m_x$	mx	Longitudinal effective mass	0.4	$m_e$
$m_y$	my	Transverse effective mass	0.4	$m_e$
$m_z$	mz	Transverse effective mass	0.4	$m_e$

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Table 619 Parameters of U-valley model (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$\alpha$	a	Valley nonparabolicity factor	0.4	—
$Z_f$	zf	Fraction of the valley within the first Brillouin zone	0.5	—

Table 620 Parameters of M-valley model

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Minima with respect to band edge	3.0	eV
$m_x$	mx	Longitudinal effective mass	0.57	$m_e$
$m_y$	my	Transverse effective mass	0.57	$m_e$
$m_z$	mz	Transverse effective mass	0.57	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$Z_f$	zf	Fraction of the valley within the first Brillouin zone	0.5	—

Table 621 Parameters of K-valley model

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Minima with respect to band edge	3.1	eV
$m_x$	mx	Longitudinal effective mass	0.3	$m_e$
$m_y$	my	Transverse effective mass	0.3	$m_e$
$m_z$	mz	Transverse effective mass	0.3	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.7	—

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Table 621 Parameters of K-valley model (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$Z_f$	zf	Fraction of the valley within the first Brillouin zone	0.333333	–

## G1-Valley Scattering Mechanisms

The  $\Gamma$ -minimum defines the set of scattering mechanisms listed in Table 622. By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL GaN.conduction.C1.<valley>.<mechanism> ADD
```

```
MATERIAL GaN.conduction.C1.<valley>.<mechanism> REMOVE
```

Table 622 Scattering mechanisms for G1-minimum

Scattering mechanism	Mechanism name
Acoustic Phonon	ac
Polar Optical Phonon	pop
Optical Phonon (inter)	opg3
Optical Phonon (inter)	opu1
Optical Phonon (inter)	opu2
Optical Phonon (inter)	opu3
Optical Phonon (inter)	opu4
Optical Phonon (inter)	opu5
Optical Phonon (inter)	opu6
Optical Phonon (inter)	opu7
Optical Phonon (inter)	opu8
Optical Phonon (inter)	opu9

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Table 622 Scattering mechanisms for G1-minimum (Continued)

Scattering mechanism	Mechanism name
Optical Phonon (inter)	opu10
Optical Phonon (inter)	opu11
Optical Phonon (inter)	opu12
Optical Phonon (inter)	opm1
Optical Phonon (inter)	opm2
Optical Phonon (inter)	opm3
Optical Phonon (inter)	opm4
Optical Phonon (inter)	opm5
Optical Phonon (inter)	opm6
Optical Phonon (inter)	opk1
Optical Phonon (inter)	opk2
Optical Phonon (inter)	opk3
Optical Phonon (inter)	opk4
Optical Phonon (inter)	opk5
Optical Phonon (inter)	opk6
Ionized Impurity	II
Surface Roughness	SR

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each  $\Gamma$ -minimum, listed in [Table 622](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL GaN.conduction.C1.<valley>.<mechanism>. <parameter> <value>
```

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### Conduction Band Model

#### Elastic Acoustic Phonon Scattering

Table 623 lists the default parameter values of intravalley elastic acoustic phonon scattering.

Table 623 Parameters of elastic acoustic phonon scattering

Parameter symbol	Parameter name	Valley name:	G1	Unit
		Mechanism name:	ac	
		Description	Default	
$\Delta_{ac}$	D	Acoustic deformation	8.3	eV
v	v	Velocity	$6.56 \times 10^3$	m/s
i	final	Final minima	G1	—

#### Optical Phonon Scattering

Table 624 to Table 627 list the default parameter values of intervalley optical phonon scattering.

Table 624 Parameters of intervalley G1 to G3 optical phonon scattering

Parameter symbol	Parameter name	Valley name:	G1	Unit
		Mechanism name:	opg3	
		Description	Default	
$E_{op}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV
$D_{op}$	Cc	Coupling constant	$1 \times 10^{11}$	eV/m
i	final	Final minima	G3	—

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### Conduction Band Model

Table 625 Parameters of intervalley G1 to U optical phonon scattering

Parameter symbol	Parameter name	Valley name:	G1	Unit
<b>Mechanism name:</b> opu[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]				
		Description	Default	
$E_{op}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV
$D_{op}$	cc	Coupling constant	$1 \times 10^{11}$	eV/m
$i$	final	Final minima	U[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]	–

Table 626 Parameters of intervalley G1 to M optical phonon scattering

Parameter symbol	Parameter name	Valley name:	G1	Unit
<b>Mechanism name:</b> opm[1, 2, 3, 4, 5, 6]				
		Description	Default	
$E_{op}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV
$D_{op}$	cc	Coupling constant	$1 \times 10^{11}$	eV/m
$i$	final	Final minima	M[1, 2, 3, 4, 5, 6]	–

Table 627 Parameters of intervalley G1 to K optical phonon scattering

Parameter symbol	Parameter name	Valley name:	G1	Unit
<b>Mechanism name:</b> opk[1, 2, 3, 4, 5, 6]				
		Description	Default	
$E_{op}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV

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Table 627 Parameters of intervalley G1 to K optical phonon scattering (Continued)

Parameter symbol	Parameter name	Valley name:	G1	Unit
		Mechanism name:	opk[1, 2, 3, 4, 5, 6]	
		Description	Default	
$D_{op}$	cc	Coupling constant	$1 \times 10^{11}$	eV/m
$i$	final	Final minima	K[1, 2, 3, 4, 5, 6]	—

### Polar-Optical Phonon Scattering

Table 628 lists the default parameter values of intravalley polar-optical phonon scattering.

Table 628 Parameters of polar-optical phonon scattering

Parameter symbol	Parameter name	Valley name:	G1	Unit
		Mechanism name:	pop	
		Description	Default	
$E_{op}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV
$i$	final	Final minima	G1	—

## G3-Valley Scattering Mechanisms

The  $\Gamma$ -minimum defines the set of scattering mechanisms listed in Table 629. By default, all these scattering mechanisms are added to the default scattering model.

To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL GaN.conduction.C2.<valley>.<mechanism> ADD
```

```
MATERIAL GaN.conduction.C2.<valley>.<mechanism> REMOVE
```

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## Conduction Band Model

*Table 629 Scattering mechanisms for G3-minimum*

Scattering mechanism	Mechanism name
Acoustic Phonon	ac
Polar Optical Phonon	pop
Optical Phonon (inter)	opg1
Optical Phonon (inter)	opu1
Optical Phonon (inter)	opu2
Optical Phonon (inter)	opu3
Optical Phonon (inter)	opu4
Optical Phonon (inter)	opu5
Optical Phonon (inter)	opu6
Optical Phonon (inter)	opu7
Optical Phonon (inter)	opu8
Optical Phonon (inter)	opu9
Optical Phonon (inter)	opu10
Optical Phonon (inter)	opu11
Optical Phonon (inter)	opu12
Optical Phonon (inter)	opm1
Optical Phonon (inter)	opm2
Optical Phonon (inter)	opm3
Optical Phonon (inter)	opm4
Optical Phonon (inter)	opm5
Optical Phonon (inter)	opm6
Optical Phonon (inter)	opk1

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Table 629 Scattering mechanisms for G3-minimum (Continued)

Scattering mechanism	Mechanism name
Optical Phonon (inter)	opk2
Optical Phonon (inter)	opk3
Optical Phonon (inter)	opk4
Optical Phonon (inter)	opk5
Optical Phonon (inter)	opk6
Ionized Impurity	II
Surface Roughness	SR

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each  $\Gamma$ -minimum, listed in [Table 629](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL GaN.conduction.C2.<valley>.<mechanism>.<parameter> <value>
```

### Elastic Acoustic Phonon Scattering

[Table 630](#) lists the default parameter values of intravalley elastic acoustic phonon scattering.

Table 630 Parameters of elastic acoustic phonon scattering

Parameter symbol	Parameter name	Valley name:	G3	Unit	
		Mechanism name: ac			
		Description Default			
$\Delta_{ac}$	D	Acoustic deformation	8.3	eV	
v	v	Velocity	$6.56 \times 10^3$	m/s	
i	final	Final minima	G3	—	

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#### Optical Phonon Scattering

[Table 631](#) to [Table 634](#) list the default parameter values of intervalley optical phonon scattering.

*Table 631 Parameters of intervalley G3 to G1 optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G3	Unit
		Mechanism name:	opg1	
		Description	Default	
$E_{\text{op}}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV
$D_{\text{op}}$	cc	Coupling constant	$1 \times 10^{11}$	eV/m
$i$	final	Final minima	G1	—

*Table 632 Parameters of intervalley G3 to U optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G3	Unit
		Mechanism name:	opu[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]	
		Description	Default	
$E_{\text{op}}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV
$D_{\text{op}}$	cc	Coupling constant	$1 \times 10^{11}$	eV/m
$i$	final	Final minima	U[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]	—

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### Conduction Band Model

*Table 633 Parameters of intervalley G3 to M optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G3	Unit
		Mechanism name:	opm[1, 2, 3, 4, 5, 6]	
		Description	Default	
$E_{\text{op}}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV
$D_{\text{op}}$	cc	Coupling constant	$1 \times 10^{11}$	eV/m
$i$	final	Final minima	M[1, 2, 3, 4, 5, 6]	—

*Table 634 Parameters of intervalley G3 to K optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G3	Unit
		Mechanism name:	opk[1, 2, 3, 4, 5, 6]	
		Description	Default	
$E_{\text{op}}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV
$D_{\text{op}}$	cc	Coupling constant	$1 \times 10^{11}$	eV/m
$i$	final	Final minima	K[1, 2, 3, 4, 5, 6]	—

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### Polar-Optical Phonon Scattering

[Table 635](#) lists the default parameter values of intravalley polar-optical phonon scattering.

*Table 635 Parameters of polar-optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	G3	Unit
		Mechanism name:	pop	
		Description	Default	
$E_{op}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV
$i$	final	Final minima	G3	-

### U-Valley Scattering Mechanisms

The 12 U-minima define the set of scattering mechanisms listed in [Table 636](#). By default, all these scattering mechanisms are added to the default scattering model. To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL GaN.conduction.C1.<valley>.<mechanism> ADD
```

```
MATERIAL GaN.conduction.C1.<valley>.<mechanism> REMOVE
```

*Table 636 Scattering mechanisms for U-minima*

Scattering mechanism	U1	U2	U3	U4	U5	U6	U7	U8	U9	U10	U11	U12
	Mechanism name											
Acoustic Phonon	ac	ac	ac	ac	ac	ac	ac	ac	ac	ac	ac	ac
Polar Optical Phonon	pop	pop	pop	pop	pop	pop	pop	pop	pop	pop	pop	pop
Optical Phonon (inter)	opg1	opg1	opg1	opg1	opg1	opg1	opg1	opg1	opg1	opg1	opg1	opg1
Optical Phonon (inter)	opg3	opg3	opg3	opg3	opg3	opg3	opg3	opg3	opg3	opg3	opg3	opg3

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Table 636 Scattering mechanisms for U-minima (Continued)

Scattering mechanism	U1	U2	U3	U4	U5	U6	U7	U8	U9	U10	U11	U12
	Mechanism name											
Optical Phonon (inter)	opu2	opu1										
Optical Phonon (inter)	opu3	opu3	opu2									
Optical Phonon (inter)	opu4	opu4	opu4	opu3								
Optical Phonon (inter)	opu5	opu5	opu5	opu5	opu4							
Optical Phonon (inter)	opu6	opu6	opu6	opu6	opu6	opu5						
Optical Phonon (inter)	opu7	opu7	opu7	opu7	opu7	opu7	opu6	opu6	opu6	opu6	opu6	opu6
Optical Phonon (inter)	opu8	opu8	opu8	opu8	opu8	opu8	opu8	opu7	opu7	opu7	opu7	opu7
Optical Phonon (inter)	opu9	opu9	opu9	opu9	opu9	opu9	opu9	opu9	opu8	opu8	opu8	opu8
Optical Phonon (inter)	opu10	opu10	opu10	opu10	opu10	opu10	opu10	opu10	opu10	opu9	opu9	opu9
Optical Phonon (inter)	opu11	opu11	opu11	opu11	opu11	opu11	opu11	opu11	opu11	opu11	opu10	opu10
Optical Phonon (inter)	opu12	opu12	opu12	opu12	opu12	opu12	opu12	opu12	opu12	opu12	opu12	opu11

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Table 636 Scattering mechanisms for U-minima (Continued)

Scattering mechanism	U1	U2	U3	U4	U5	U6	U7	U8	U9	U10	U11	U12
	Mechanism name											
Optical Phonon (inter)	opm1	opm1	opm1	opm1	opm1	opm1	opm1	opm1	opm1	opm1	opm1	opm1
Optical Phonon (inter)	opm2	opm2	opm2	opm2	opm2	opm2	opm2	opm2	opm2	opm2	opm2	opm2
Optical Phonon (inter)	opm3	opm3	opm3	opm3	opm3	opm3	opm3	opm3	opm3	opm3	opm3	opm3
Optical Phonon (inter)	opm4	opm4	opm4	opm4	opm4	opm4	opm4	opm4	opm4	opm4	opm4	opm4
Optical Phonon (inter)	opm5	opm5	opm5	opm5	opm5	opm5	opm5	opm5	opm5	opm5	opm5	opm5
Optical Phonon (inter)	opm6	opm6	opm6	opm6	opm6	opm6	opm6	opm6	opm6	opm6	opm6	opm6
Optical Phonon (inter)	opk1	opk1	opk1	opk1	opk1	opk1	opk1	opk1	opk1	opk1	opk1	opk1
Optical Phonon (inter)	opk2	opk2	opk2	opk2	opk2	opk2	opk2	opk2	opk2	opk2	opk2	opk2
Optical Phonon (inter)	opk3	opk3	opk3	opk3	opk3	opk3	opk3	opk3	opk3	opk3	opk3	opk3
Optical Phonon (inter)	opk4	opk4	opk4	opk4	opk4	opk4	opk4	opk4	opk4	opk4	opk4	opk4
Optical Phonon (inter)	opk5	opk5	opk5	opk5	opk5	opk5	opk5	opk5	opk5	opk5	opk5	opk5

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Table 636 Scattering mechanisms for U-minima (Continued)

Scattering mechanism	U1	U2	U3	U4	U5	U6	U7	U8	U9	U10	U11	U12
	Mechanism name											
Optical Phonon (inter)	opk6	opk6	opk6	opk6	opk6	opk6	opk6	opk6	opk6	opk6	opk6	opk6
Ionized Impurity	II	II	II	II	II	II	II	II	II	II	II	II
Surface Roughness	SR	SR	SR	SR	SR	SR	SR	SR	SR	SR	SR	SR

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each U-minimum, listed in Table 636, have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL GaN.conduction.C1.<valley>.<mechanism>. <parameter> <value>
```

### Elastic Acoustic Phonon Scattering

Table 637 lists the default parameter values of intravalley elastic acoustic phonon scattering.

Table 637 Parameters of elastic acoustic phonon scattering

Parameter symbol	Parameter name	Valley name:	U[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]	Unit
		Mechanism name:	ac	
		Description	Default	
$\Delta_{ac}$	D	Acoustic deformation	8.3	eV
$v$	v	Velocity	$6.56 \times 10^3$	m/s
$i$	final	Final minima	U[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]	–

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#### Optical Phonon Scattering

Table 638 to Table 641 list the default parameter values of intervalley optical phonon scattering.

Table 638 Parameters of intervalley U to G1 optical phonon scattering

Parameter symbol	Parameter name	Valley name:	U[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]	Unit
		Mechanism name:	opg1	
		Description	Default	
$E_{\text{op}}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV
$D_{\text{op}}$	cc	Coupling constant	$1 \times 10^{11}$	eV/m
$i$	final	Final minima	G1	—

Table 639 Parameters of intervalley U to G3 optical phonon scattering

Parameter symbol	Parameter name	Valley name:	U[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]	Unit
		Mechanism name:	opg3	
		Description	Default	
$E_{\text{op}}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV
$D_{\text{op}}$	cc	Coupling constant	$1 \times 10^{11}$	eV/m
$i$	final	Final minima	G3	—

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*Table 640 Parameters of intervalley U to M optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	U[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]	Unit
		Mechanism name:	opm[1, 2, 3, 4, 5, 6]	
		Description	Default	
$E_{\text{op}}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV
$D_{\text{op}}$	cc	Coupling constant	$1 \times 10^{11}$	eV/m
$i$	final	Final minima	M[1, 2, 3, 4, 5, 6]	—

*Table 641 Parameters of intervalley U to K optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	U[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]	Unit
		Mechanism name:	opk[1, 2, 3, 4, 5, 6]	
		Description	Default	
$E_{\text{op}}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV
$D_{\text{op}}$	cc	Coupling constant	$1 \times 10^{11}$	eV/m
$i$	final	Final minima	K[1, 2, 3, 4, 5, 6]	—

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

#### Polar-Optical Phonon Scattering

Table 642 lists the default parameter values of intravalley polar-optical phonon scattering.

Table 642 Parameters of polar-optical phonon scattering

Parameter symbol	Parameter name	Valley name:	U[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]	Unit
		Mechanism name:	pop	
		Description	Default	
$E_{op}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV
$i$	final	Final minima	U[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]	—

#### M-Valley Scattering Mechanisms

The six M-minima define the set of scattering mechanisms listed in Table 643. By default, all these scattering mechanisms are added to the default scattering model. To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL GaN.conduction.C1.<valley>.<mechanism> ADD
```

```
MATERIAL GaN.conduction.C1.<valley>.<mechanism> REMOVE
```

Table 643 Scattering mechanisms for M-minima

Scattering mechanism	M1	M2	M3	M4	M5	M6
	Mechanism name					
Acoustic Phonon	ac	ac	ac	ac	ac	ac
Polar Optical Phonon	pop	pop	pop	pop	pop	pop
Optical Phonon (inter)	opg1	opg1	opg1	opg1	opg1	opg1
Optical Phonon (inter)	opg3	opg3	opg3	opg3	opg3	opg3
Optical Phonon (inter)	opu1	opu1	opu1	opu1	opu1	opu1
Optical Phonon (inter)	opu2	opu2	opu2	opu2	opu2	opu2
Optical Phonon (inter)	opu3	opu3	opu3	opu3	opu3	opu3

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## Conduction Band Model

*Table 643 Scattering mechanisms for M-minima (Continued)*

Scattering mechanism	M1	M2	M3	M4	M5	M6
	Mechanism name					
Optical Phonon (inter)	opu4	opu4	opu4	opu4	opu4	opu4
Optical Phonon (inter)	opu5	opu5	opu5	opu5	opu5	opu5
Optical Phonon (inter)	opu6	opu6	opu6	opu6	opu6	opu6
Optical Phonon (inter)	opu7	opu7	opu7	opu7	opu7	opu7
Optical Phonon (inter)	opu8	opu8	opu8	opu8	opu8	opu8
Optical Phonon (inter)	opu9	opu9	opu9	opu9	opu9	opu9
Optical Phonon (inter)	opu10	opu10	opu10	opu10	opu10	opu10
Optical Phonon (inter)	opu11	opu11	opu11	opu11	opu11	opu11
Optical Phonon (inter)	opu12	opu12	opu12	opu12	opu12	opu12
Optical Phonon (inter)	opm2	opm1	opm1	opm1	opm1	opm1
Optical Phonon (inter)	opm3	opm3	opm2	opm2	opm2	opm2
Optical Phonon (inter)	opm4	opm4	opm4	opm3	opm3	opm3
Optical Phonon (inter)	opm5	opm5	opm5	opm5	opm4	opm4
Optical Phonon (inter)	opm6	opm6	opm6	opm6	opm6	opm5
Optical Phonon (inter)	opk1	opk1	opk1	opk1	opk1	opk1
Optical Phonon (inter)	opk2	opk2	opk2	opk2	opk2	opk2
Optical Phonon (inter)	opk3	opk3	opk3	opk3	opk3	opk3
Optical Phonon (inter)	opk4	opk4	opk4	opk4	opk4	opk4
Optical Phonon (inter)	opk5	opk5	opk5	opk5	opk5	opk5
Optical Phonon (inter)	opk6	opk6	opk6	opk6	opk6	opk6

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

Table 643 Scattering mechanisms for M-minima (Continued)

Scattering mechanism	M1	M2	M3	M4	M5	M6
Mechanism name						
Ionized Impurity	II	II	II	II	II	II
Surface Roughness	SR	SR	SR	SR	SR	SR

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each M-minimum, listed in [Table 643](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL GaN.conduction.C1.<valley>.<mechanism>.<parameter> <value>
```

### Elastic Acoustic Phonon Scattering

[Table 644](#) lists the default parameter values of intravalley elastic acoustic phonon scattering.

Table 644 Parameters of elastic acoustic phonon scattering

Parameter symbol	Parameter name	Valley name:	M[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	ac	
		Description	Default	
$\Delta_{ac}$	D	Acoustic deformation	8.3	eV
$v$	v	Velocity	$6.56 \times 10^3$	m/s
$i$	final	Final minima	M[1, 2, 3, 4, 5, 6]	—

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

#### Optical Phonon Scattering

Table 645 to Table 648 list the default parameter values of intervalley optical phonon scattering.

Table 645 Parameters of intervalley M to G1 optical phonon scattering

Parameter symbol	Parameter name	Valley name:	M[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	opg1	
		Description	Default	
$E_{\text{op}}$	$E$	Phonon energy	$91.2 \times 10^{-3}$	eV
$D_{\text{op}}$	$cc$	Coupling constant	$1 \times 10^{11}$	eV/m
$i$	$\text{final}$	Final minima	G1	—

Table 646 Parameters of intervalley M to G3 optical phonon scattering

Parameter symbol	Parameter name	Valley name:	M[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	opg3	
		Description	Default	
$E_{\text{op}}$	$E$	Phonon energy	$91.2 \times 10^{-3}$	eV
$D_{\text{op}}$	$cc$	Coupling constant	$1 \times 10^{11}$	eV/m
$i$	$\text{final}$	Final minima	G3	—

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

*Table 647 Parameters of intervalley M to U optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	M[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	opu[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]	
		Description	Default	
$E_{\text{op}}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV
$D_{\text{op}}$	Cc	Coupling constant	$1 \times 10^{11}$	eV/m
$i$	final	Final minima	U[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]	—

*Table 648 Parameters of intervalley M to K optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	M[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	opk[1, 2, 3, 4, 5, 6]	
		Description	Default	
$E_{\text{op}}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV
$D_{\text{op}}$	Cc	Coupling constant	$1 \times 10^{11}$	eV/m
$i$	final	Final minima	K[1, 2, 3, 4, 5, 6]	—

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

#### Polar-Optical Phonon Scattering

Table 649 lists the default parameter values of intravalley polar-optical phonon scattering.

Table 649 Parameters of polar-optical phonon scattering

Parameter symbol	Parameter name	Valley name:	M[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	pop	
		Description	Default	
$E_{op}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV
i	final	Final minima	M[1, 2, 3, 4, 5, 6]	—

#### K-Valley Scattering Mechanisms

The six K-minima define the set of scattering mechanisms listed in Table 650. By default, all these scattering mechanisms are added to the default scattering model. To change the default scattering model by adding or removing defined scattering mechanisms, use the following input file syntax:

```
MATERIAL GaN.conduction.C1.<valley>.<mechanism> ADD
```

```
MATERIAL GaN.conduction.C1.<valley>.<mechanism> REMOVE
```

Table 650 Scattering mechanisms for K-minima

Scattering mechanism	K1	K2	K3	K4	K5	K6
	Mechanism name					
Acoustic Phonon	ac	ac	ac	ac	ac	ac
Polar Optical Phonon	pop	pop	pop	pop	pop	pop
Optical Phonon (inter)	opg1	opg1	opg1	opg1	opg1	opg1
Optical Phonon (inter)	opg3	opg3	opg3	opg3	opg3	opg3
Optical Phonon (inter)	opu1	opu1	opu1	opu1	opu1	opu1
Optical Phonon (inter)	opu2	opu2	opu2	opu2	opu2	opu2
Optical Phonon (inter)	opu3	opu3	opu3	opu3	opu3	opu3

**Chapter 25: Gallium Nitride Material Model**

## Conduction Band Model

*Table 650 Scattering mechanisms for K-minima (Continued)*

Scattering mechanism	K1	K2	K3	K4	K5	K6
	Mechanism name					
Optical Phonon (inter)	opu4	opu4	opu4	opu4	opu4	opu4
Optical Phonon (inter)	opu5	opu5	opu5	opu5	opu5	opu5
Optical Phonon (inter)	opu6	opu6	opu6	opu6	opu6	opu6
Optical Phonon (inter)	opu7	opu7	opu7	opu7	opu7	opu7
Optical Phonon (inter)	opu8	opu8	opu8	opu8	opu8	opu8
Optical Phonon (inter)	opu9	opu9	opu9	opu9	opu9	opu9
Optical Phonon (inter)	opu10	opu10	opu10	opu10	opu10	opu10
Optical Phonon (inter)	opu11	opu11	opu11	opu11	opu11	opu11
Optical Phonon (inter)	opu12	opu12	opu12	opu12	opu12	opu12
Optical Phonon (inter)	opm1	opm1	opm1	opm1	opm1	opm1
Optical Phonon (inter)	opm2	opm2	opm2	opm2	opm2	opm2
Optical Phonon (inter)	opm3	opm3	opm3	opm3	opm3	opm3
Optical Phonon (inter)	opm4	opm4	opm4	opm4	opm4	opm4
Optical Phonon (inter)	opm5	opm5	opm5	opm5	opm5	opm5
Optical Phonon (inter)	opm6	opm6	opm6	opm6	opm6	opm6
Optical Phonon (inter)	opk2	opk1	opk1	opk1	opk1	opk1
Optical Phonon (inter)	opk3	opk3	opk2	opk2	opk2	opk2
Optical Phonon (inter)	opk4	opk4	opk4	opk3	opk3	opk3
Optical Phonon (inter)	opk5	opk5	opk5	opk5	opk4	opk4
Optical Phonon (inter)	opk6	opk6	opk6	opk6	opk6	opk5

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

*Table 650 Scattering mechanisms for K-minima (Continued)*

Scattering mechanism	K1	K2	K3	K4	K5	K6
<b>Mechanism name</b>						
Ionized Impurity	II	II	II	II	II	II
Surface Roughness	SR	SR	SR	SR	SR	SR

## Parameters of Scattering Mechanisms

By default, the equivalent scattering mechanisms defined for each K-minimum, listed in [Table 650](#), have the same parameter values.

To change these parameter values, use the following input file syntax:

```
MATERIAL GaN.conduction.C1.<valley>.<mechanism>.<parameter> <value>
```

### Elastic Acoustic Phonon Scattering

[Table 651](#) lists the default parameter values of intravalley elastic acoustic phonon scattering.

*Table 651 Parameters of elastic acoustic phonon scattering*

Parameter symbol	Parameter name	Valley name:	K[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	ac	
		Description	Default	
$\Delta_{ac}$	D	Acoustic deformation	8.3	eV
$v$	v	Velocity	$6.56 \times 10^3$	m/s
$i$	final	Final minima	K[1, 2, 3, 4, 5, 6]	—

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

#### Optical Phonon Scattering

Table 652 to Table 655 list the default parameter values of intervalley optical phonon scattering.

Table 652 Parameters of intervalley K to G1 optical phonon scattering

Parameter symbol	Parameter name	Valley name:	K[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	opg1	
		Description	Default	
$E_{\text{op}}$	$E$	Phonon energy	$91.2 \times 10^{-3}$	eV
$D_{\text{op}}$	$cc$	Coupling constant	$1 \times 10^{11}$	eV/m
$i$	$\text{final}$	Final minima	G1	—

Table 653 Parameters of intervalley K to G3 optical phonon scattering

Parameter symbol	Parameter name	Valley name:	K[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	opg3	
		Description	Default	
$E_{\text{op}}$	$E$	Phonon energy	$91.2 \times 10^{-3}$	eV
$D_{\text{op}}$	$cc$	Coupling constant	$1 \times 10^{11}$	eV/m
$i$	$\text{final}$	Final minima	G3	—

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

*Table 654 Parameters of intervalley K to U optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	K[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	opu[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]	
		Description	Default	
$E_{\text{op}}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV
$D_{\text{op}}$	Cc	Coupling constant	$1 \times 10^{11}$	eV/m
$i$	final	Final minima	U[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]	—

*Table 655 Parameters of intervalley K to M optical phonon scattering*

Parameter symbol	Parameter name	Valley name:	K[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	opm[1, 2, 3, 4, 5, 6]	
		Description	Default	
$E_{\text{op}}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV
$D_{\text{op}}$	Cc	Coupling constant	$1 \times 10^{11}$	eV/m
$i$	final	Final minima	M[1, 2, 3, 4, 5, 6]	—

## Chapter 25: Gallium Nitride Material Model

### Conduction Band Model

#### Polar-Optical Phonon Scattering

Table 656 lists the default parameter values of intravalley polar-optical phonon scattering.

Table 656 Parameters of polar-optical phonon scattering

Parameter symbol	Parameter name	Valley name:	K[1, 2, 3, 4, 5, 6]	Unit
		Mechanism name:	pop	
		Description	Default	
$E_{op}$	E	Phonon energy	$91.2 \times 10^{-3}$	eV
$i$	final	Final minima	K[1, 2, 3, 4, 5, 6]	—

#### Ionized Impurity Scattering

Ionized impurity scattering is defined for each valley in a conduction band and is treated as an intravalley process by default, so that the final valley after scattering is the same as the initial valley.

Table 657 Parameters of ionized impurity scattering

Parameter symbol	Parameter name	Valley name:	All valleys	Unit
		Mechanism name:	II	
		Description	Default	
$i$	final	Final minimum	Same as initial minimum	—

#### Ionized Impurity Empirical Rate Factor

The ionized impurity scattering model includes a scaling factor for the empirical correction of the calculated scattering rate as a function of doping density.

To redefine the default empirical factor, use the following input file syntax:

```
MATERIAL GaN.conduction.IIfac N <Nvalue> [<Nvalue2>] <rule> <value>
```

Here, **IIfac** is a piecewise interpolation parameter that defines a correction factor **<value>** for a value **<Nvalue>** of the doping concentration **N**. The interpolation model used to return values between specified densities is given by **<rule>**, which might require an upper bound of the density [**<Nvalue2>**]. For a description of the interpolation parameter type, see [Interpolation Methods on page 301](#).

## Chapter 25: Gallium Nitride Material Model

### Valence Band Model

By default, the empirical correction for ionized impurity is 1.0.

---

## Surface Roughness Scattering

[Table 658](#) lists the default parameter values of surface roughness scattering. These parameters apply to all valleys and to all equivalent surface orientations.

*Table 658 Parameters of surface roughness scattering*

Parameter symbol	Parameter name	Valley name:	All valleys	Unit
Mechanism name:				SR
Description				Default
$\Delta$	rms	RMS amplitude	0.33	nm
$L_c$	l	Correlation length	1.00	nm

---

## Valence Band Model

This section describes the valence band model.

---

## Band Edge Parameters

To change the default parameter values of the valence band container model, listed in [Table 659](#), use the following input file syntax:

```
MATERIAL GaN.valence.<parameter> <value>
```

*Table 659 Parameters of valence band container model*

Parameter symbol	Parameter name	Description	Default	Unit
$E$	E	Valence band energy with respect to vacuum	7.39544	eV
$m_{dg_x}$	dgx	Hole density gradient effective x-mass	0.5	$m_e$
$m_{dg_y}$	dgy	Hole density gradient effective y-mass	0.5	$m_e$
$m_{dg_z}$	dgz	Hole density gradient effective z-mass	0.5	$m_e$

## Chapter 25: Gallium Nitride Material Model

### Valence Band Model

To change the default parameter values of the valence bands in the container model, listed in [Table 660](#), use the following input file syntax:

```
MATERIAL GaN.valence.<band>.<parameter> <value>
```

*Table 660 Parameters of valence band model*

Parameter symbol	Parameter name	Description	Default	Unit
<b>Heavy hole (HH) band</b>				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.0	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	ema	—
<b>Light hole (LH) band</b>				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.0	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	ema	—
<b>Spin split-off (SSO) band</b>				
<i>E</i>	<i>E</i>	Valence band energy with respect to container energy	0.017	eV
<i>model</i>	<i>model</i>	Model used for transport in this band	ema	—

## Mobility Models

The valence band model defines a mobility model consisting of low field, perpendicular field, and velocity saturation mobility models.

### Low Field: Constant Mobility Model

To change the default parameter values of the constant mobility model, listed in [Table 661](#), use the following input file syntax:

```
MATERIAL GaN.valence.constant.<parameter> <value>
```

## Chapter 25: Gallium Nitride Material Model

### Valence Band Model

Table 661 Parameters of constant mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_0$	mu0	Constant low-field mobility	150	cm <sup>2</sup> /Vs
$\zeta$	zeta	Fitting parameter	2.1	—

## Low Field: Arora Mobility Model

To change the default parameter values of the Arora concentration-dependent mobility model, listed in [Table 662](#), use the following input file syntax:

```
MATERIAL GaN.valence.Arora.<parameter> <value>
```

Table 662 Parameters of Arora mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min}$	mumin	Minimum mobility	1	cm <sup>2</sup> /Vs
$\mu_{\max}$	muemax	Maximum mobility	150	cm <sup>2</sup> /Vs
$N_0$	n0	Reference concentration	$7 \times 10^{16}$	cm <sup>-3</sup>
$\alpha$	alpha	Fitting parameter	0.9	—
$\beta_1$	b1	Fitting parameter	-0.57	—
$\beta_2$	b2	Fitting parameter	-2.23	—
$\beta_3$	b3	Fitting parameter	2.40	—
$\beta_4$	b4	Fitting parameter	-0.146	—

## Low Field: Masetti Mobility Model

To change the default parameter values of the Masetti concentration-dependent mobility model, listed in [Table 663](#), use the following input file syntax:

```
MATERIAL GaN.valence.Masetti.<parameter> <value>
```

## Chapter 25: Gallium Nitride Material Model

### Valence Band Model

Table 663 Parameters of Masetti mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$\mu_{\min 1}$	mumin1	Minimum mobility	1	cm <sup>2</sup> /Vs
$\mu_{\min 2}$	mumin2	Minimum mobility	0	cm <sup>2</sup> /Vs
$\mu_{\max}$	mumax	Maximum mobility	150	cm <sup>2</sup> /Vs
$\mu_1$	mul	Maximum mobility	0	cm <sup>2</sup> /Vs
$C_r$	cr	Reference concentration	$9.5 \times 10^{16}$	cm <sup>-3</sup>
$C_s$	cs	Reference solid solubility concentration	$1 \times 10^{16}$	cm <sup>-3</sup>
$p_c$	pc	Reference concentration	$5 \times 10^{18}$	cm <sup>-3</sup>
$\alpha$	alpha	Fitting parameter	0.9	—
$\beta$	beta	Fitting parameter	0.9	—
$\zeta$	zeta	Fitting parameter	2.1	—

## Perpendicular Field: Yamaguchi Mobility Model

To change the default parameter values of the Yamaguchi mobility model, listed in [Table 664](#), use the following input file syntax:

```
MATERIAL GaN.valence.Yamaguchi.<parameter> <value>
```

Table 664 Parameters of Yamaguchi mobility model

Parameter symbol	Parameter name	Description	Default	Unit
$E_c$	ec	Critical field	$5 \times 10^5$	V/cm
$\alpha$	alpha	Fitting parameter	1.0	—

## Chapter 25: Gallium Nitride Material Model

### Valence Band Model

## High Field: Caughey–Thomas Velocity Saturation Mobility Model

To change the default parameter values of the Caughey–Thomas velocity saturation mobility model, listed in [Table 665](#), use the following input file syntax:

```
MATERIAL GaN.valence.Caughey.<parameter> <value>
```

*Table 665 Parameters of Caughey–Thomas mobility model*

Parameter symbol	Parameter name	Description	Default	Unit
$v_{\text{sat}}$	vsat	Saturation velocity	$1 \times 10^7$	cm/s
$v_{\text{exp}}$	vexp	Fitting parameter	1.7	–
$\beta_0$	beta0	Fitting parameter	1	–
$\beta_{\text{exp}}$	bexp	Fitting parameter	1	–
$\alpha$	alpha	Fitting parameter	0	–

## Default Mobility Model

The default mobility model, combining low-field, perpendicular-field, and high-field mobility models, is given in [Table 666](#). To change the default mobility model, use the following input file syntax:

```
MATERIAL GaN.valence.mobility.<model> <value>
```

*Table 666 Parameters of default mobility model*

Model name	Description	Default
bulk	Sets the bulk low-field mobility model.	constant
eprp	Sets the perpendicular field–dependent mobility model.	none
elat	Sets the velocity saturation mobility model.	none

## Valley Minima

The analytic multivalley valence band model consists of the valley minima listed in [Table 667](#). To change the default model by removing valleys, use the following input file syntax:

```
MATERIAL GaN.valence.<band>.<valley> REMOVE
```

**Note:**

The valence band analytic valley approximation is used only as a way to define density-of-states for drift-diffusion simulations and to define the valley minima in response to stress.

*Table 667 Names of valence band minima*

Valence band minima	Band name	Valley name
Heavy hole	HH	vhh
Light hole	LH	vlh
Spin split-off	SSO	vsso

## Position and Orientation

The position and orientation of the HH, LH, and SSO valley minima are identical. [Table 668](#) shows the default values. To change the default values, use the following input file syntax:

```
MATERIAL GaN.valence.<band>.<valley>.min.<parameter> <value>
```

*Table 668 Position and orientation parameters of HH, LH, and SSO valley minima*

Parameter symbol	Parameter name	Description	Default	Unit
$k_0$	pos	Position within the Brillouin zone	0.0 0.0 0.0	$2\pi/\sqrt{3}a$ , $4\pi/3b$ , $2\pi/c$
$x$	x	Orientation of the x-axis	0 0 0 1	$\langle hki \rangle$
$y$	y	Orientation of the y-axis	2 -1 -1 0	$\langle hki \rangle$
$z$	z	Orientation of the z-axis	0 1 -1 0	$\langle hki \rangle$

## Chapter 25: Gallium Nitride Material Model

### Valence Band Model

## Parameters

To change the valley minima model parameters, listed in [Table 669](#), for each valley listed in [Table 667](#), use the following input file syntax:

```
MATERIAL GaN.valence.<band>.<valley>.<parameter> <value>
```

*Table 669 Parameters of valence band minima*

Parameter symbol	Parameter name	Description	Default	Unit
<b>Heavy hole (HH) band</b>				
$E$	E	Minima with respect to band edge	0.0	eV
$m_x$	mx	Longitudinal effective mass	1.89	$m_e$
$m_y$	my	Transverse effective mass	0.29	$m_e$
$m_z$	mz	Transverse effective mass	0.29	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	0.0	eV
<b>Light hole (LH) band</b>				
$E$	E	Minima with respect to band edge	0.0	eV
$m_x$	mx	Longitudinal effective mass	0.44	$m_e$
$m_y$	my	Transverse effective mass	0.39	$m_e$
$m_z$	mz	Transverse effective mass	0.39	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	0.0	eV
<b>Spin split-off (SSO) band</b>				
$E$	E	Minima with respect to band edge	0.0	eV

## Chapter 25: Gallium Nitride Material Model

### Valence Band Model

Table 669 Parameters of valence band minima (Continued)

Parameter symbol	Parameter name	Description	Default	Unit
$m_x$	mx	Longitudinal effective mass	0.18	$m_e$
$m_y$	my	Transverse effective mass	1.05	$m_e$
$m_z$	mz	Transverse effective mass	1.05	$m_e$
$\alpha$	a	Valley nonparabolicity factor	0.0	—
$a_v$	av	Hydrostatic deformation potential	0.0	eV

---

## Heavy-Hole Band Scattering Mechanisms

There are no heavy-hole band scattering mechanisms defined in the current version of Garand.

---

## Light-Hole Band Scattering Mechanisms

There are no light-hole band scattering mechanisms defined in the current version of Garand.

---

## Spin Split-Off Band Scattering Mechanisms

There are no spin split-off band scattering mechanisms defined in the current version of Garand.

## **Part V: Appendices**

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This part of the *Garand User Guide* contains the following appendices:

- [Appendix A, Garand Materials](#)
- [Appendix B, Input File Commands](#)
- [Appendix C, Deprecated Input Commands](#)

# A

## Garand Materials

---

*This appendix lists the materials available in Garand and the names to use when referring to these materials in a Garand input file.*

---

### Semiconductor Materials

Table 670 Semiconductor materials

Material	Garand name	Material	Garand name
Silicon	Silicon	In <sub>0.6</sub> Al <sub>0.4</sub> As	In60Al40As*
Germanium	Germanium	In <sub>0.5</sub> Al <sub>0.5</sub> As	In50Al50As*
Silicon germanium	SiliconGermanium*	In <sub>0.4</sub> Al <sub>0.6</sub> As	In40Al60As*
Si <sub>0.9</sub> Ge <sub>0.1</sub>	Si90Ge10*	In <sub>0.3</sub> Al <sub>0.7</sub> As	In30Al70As*
Si <sub>0.8</sub> Ge <sub>0.2</sub>	Si80Ge20*	In <sub>0.2</sub> Al <sub>0.8</sub> As	In20Al80As*
Si <sub>0.7</sub> Ge <sub>0.3</sub>	Si70Ge30*	In <sub>0.1</sub> Al <sub>0.9</sub> As	In10Al90As*
Si <sub>0.6</sub> Ge <sub>0.4</sub>	Si60Ge40*	In <sub>0.52</sub> Al <sub>0.48</sub> As	In52Al48As_fixed
Si <sub>0.5</sub> Ge <sub>0.5</sub>	Si50Ge50*	Indium gallium arsenide	InGaAs†
Si <sub>0.4</sub> Ge <sub>0.6</sub>	Si40Ge60*	In <sub>0.9</sub> Ga <sub>0.1</sub> As	In90Ga10As*
Si <sub>0.3</sub> Ge <sub>0.7</sub>	Si30Ge70*	In <sub>0.8</sub> Ga <sub>0.2</sub> As	In80Ga20As*
Si <sub>0.2</sub> Ge <sub>0.8</sub>	Si20Ge80*	In <sub>0.7</sub> Ga <sub>0.3</sub> As	In70Ga30As*

## Appendix A: Garand Materials

### Insulator Materials

Table 670 Semiconductor materials (Continued)

Material	Garand name	Material	Garand name
$\text{Si}_{0.1}\text{Ge}_{0.9}$	$\text{Si10Ge90}^*$	$\text{In}_{0.6}\text{Ga}_{0.4}\text{As}$	$\text{In60Ga40As}^*$
Aluminum arsenide	$\text{AlAs}$	$\text{In}_{0.5}\text{Ga}_{0.5}\text{As}$	$\text{In50Ga50As}^*$
Gallium arsenide	$\text{GaAs}$	$\text{In}_{0.4}\text{Ga}_{0.6}\text{As}$	$\text{In40Ga60As}^*$
Indium arsenide	$\text{InAs}$	$\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$	$\text{In30Ga70As}^*$
Indium aluminum arsenide	$\text{InAlAs}^{\dagger}$	$\text{In}_{0.2}\text{Ga}_{0.8}\text{As}$	$\text{In20Ga80As}^*$
$\text{In}_{0.9}\text{Al}_{0.1}\text{As}$	$\text{In90Al10As}^*$	$\text{In}_{0.1}\text{Ga}_{0.9}\text{As}$	$\text{In10Ga90As}^*$
$\text{In}_{0.8}\text{Al}_{0.2}\text{As}$	$\text{In80Al20As}^*$	$\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$	$\text{In53Ga47As\_fixed}$
$\text{In}_{0.7}\text{Al}_{0.3}\text{As}$	$\text{In70Al30As}^*$		

\* These binary materials are derived using interpolation formulas. Therefore, when changing material parameters, specify an interpolator. Otherwise, the value is set for all alloy fractions.

† These binary materials are generic placeholders and are replaced in the simulation by the nearest 10% fractional material depending on the value of the `xMoleFraction` field. Changing material parameters for one of these materials modifies all fractions of the material (including root materials). Therefore, you must specify an interpolator.

---

## Insulator Materials

Table 671 Insulator materials

Material	Garand name	Material	Garand name
Air	Air   Gas   Void	Silicon dioxide ( $\text{SiO}_2$ )	GenericOxide1*
Silicon dioxide ( $\text{SiO}_2$ )	Oxide	Silicon dioxide ( $\text{SiO}_2$ )	GenericOxide2*
Buried oxide ( $\text{SiO}_2$ )	BuriedOxide	Silicon dioxide ( $\text{SiO}_2$ )	GenericOxide3*
Interfacial oxide ( $\text{SiO}_2$ )	InterfacialOxide	Silicon dioxide ( $\text{SiO}_2$ )	GenericOxide4*

## Appendix A: Garand Materials

### Insulator Materials

Table 671 Insulator materials (Continued)

Material	Garand name	Material	Garand name
Hafnium oxide ( $\text{HfO}_2$ )	HfO2	Silicon dioxide ( $\text{SiO}_2$ )	GenericOxide5*
Silicon oxynitride	Oxynitride	Silicon dioxide ( $\text{SiO}_2$ )	GenericOxide6*
Silicon nitride	Nitride	Silicon dioxide ( $\text{SiO}_2$ )	GenericOxide7*
Low-k dielectric	LowK	Silicon dioxide ( $\text{SiO}_2$ )	GenericOxide8*
Aluminum oxide ( $\text{Al}_2\text{O}_3$ )	Al2O3	Silicon dioxide ( $\text{SiO}_2$ )	GenericOxide9*
Photoresist, Mask	Photoresist		

\* Generic oxides are copies of the  $\text{SiO}_2$  material that can be used as substitutes for different insulators in the TDR file, and then their properties can be modified as required.

# B

## **Input File Commands**

---

*This appendix presents the input file commands used by Garand and Garand MC.*

---

### **Command Syntax**

All inputs have the same basic syntax as follows:

<command> <parameter>=<value>

Inputs must always be on one line, and there can be only one specified per line.

**Note:**

Some parameters accept comma-separated lists of values. In those cases, do not insert space between values and commas.

In this appendix, a backslash indicates a line continuation of commands for the purposes of formatting only.

## Appendix B: Input File Commands

automesh command

---

### automesh command

This command allows a mesh to be specified automatically when using Garand (see [Automatically Specifying a Mesh on page 56](#)).

#### Syntax

```
automesh <option> <parameter>=<value> <parameter>=<value> ...
```

Parameter	Description	Default	Unit
<option>	Specifies either to identify the channel based on a bounding material or to create a mesh along a given direction. Options are: <ul style="list-style-type: none"><li>• channel</li><li>• x</li><li>• y</li><li>• z</li></ul>	–	–
block=<integer>	Sets the index of the block of material, specified by <code>mat</code> , that is used to define the transition at which the key mesh point will be added.	–	–
block2=<integer>	Sets the index of the optional second block of material specified by <code>mat2</code> . If specified, then the key mesh point is added at the midpoint between the material transitions defined by <code>mat/block</code> and <code>mat2/block2</code> .	–	–
dh=<float>	Sets the mesh spacing at the specified key mesh point.	–	Input unit <sup>1</sup>
dh_xstart=<float>	Sets the initial mesh spacing along the x-direction (channel specification only).	–	Input unit <sup>1</sup>
dh_xmid=<float>	Sets the midpoint mesh spacing along the x-direction (channel specification only).	–	Input unit <sup>1</sup>
dh_xend=<float>	Sets the final mesh spacing along the x-direction (channel specification only).	–	Input unit <sup>1</sup>
dh_ystart=<float>	Sets the initial mesh spacing along the y-direction (channel specification only).	–	Input unit <sup>1</sup>
dh_ymid=<float>	Sets the midpoint mesh spacing along the y-direction (channel specification only).	–	Input unit <sup>1</sup>

## Appendix B: Input File Commands

### automesh command

Parameter	Description	Default	Unit
dh_yend=<float>	Sets the final mesh spacing along the y-direction (channel specification only).	–	Input unit <sup>1</sup>
dh_zstart=<float>	Sets the initial mesh spacing along the z-direction (channel specification only).	–	Input unit <sup>1</sup>
dh_zmid=<float>	Sets the midpoint mesh spacing along the z-direction (channel specification only).	–	Input unit <sup>1</sup>
dh_zend=<float>	Sets the final mesh spacing along the z-direction (channel specification only).	–	Input unit <sup>1</sup>
mat=<string>	Sets either the bounding material for channel identification or the material in the block used to define the material transition at which a key mesh point is added, along a specified direction.	–	–
mat2=<string>	Sets the material in an optional second block used to define a second material transition. If specified, then the key mesh point is added at the midpoint between the material transitions defined by mat/block and mat2/block2.	–	–
offset=<float>	Adds an offset to the detected material transition at which the key mesh point is added.	–	Input unit <sup>1</sup>
transition=<string>	Specifies whether the material transition used to define the key mesh point is at the start or the end of the block of material defined by mat/block. Options are: <ul style="list-style-type: none"> <li>• start</li> <li>• end</li> </ul>	–	–
transition2=<string>	Specifies whether the optional second material transition is at the start or the end of the block of material defined by mat2/block2. Options are: <ul style="list-style-type: none"> <li>• start</li> <li>• end</li> </ul>	–	–

1. The default input unit for Garand is the nanometer, but it can be changed (see Dimensional Unit on page 45).

## Appendix B: Input File Commands

### bias Command

---

## bias Command

This command controls the applied voltages and associated parameters in Garand (see [Bias Conditions on page 98](#)).

#### Note:

This command applies only to Garand.

#### Syntax

```
bias <parameter>=<value>
```

Parameter	Description	Default	Unit
delta=<float>	Sets the change in gate or drain bias to be applied at each step of the I–V curve, depending on the setting of simulation sim_type. It is used only if the dependent variable in the I–V curve has not been specified as a comma-separated list.  In general, it should be positive for NMOS devices and negative for PMOS devices.	0.1	V
drain=<float>   <list>	Sets the initial drain bias to apply as either a single value or a comma-separated list of values.  In general, it should be positive for NMOS devices and negative for PMOS devices.	–	V
gate=<float>   <list>	Sets the initial gate bias to apply as either a single value or a comma-separated list of values.  In general, it should be positive for NMOS devices and negative for PMOS devices, unless the device is operating in accumulation mode.	–	V
ivpoints=<integer>	Sets the number of I–V points to simulate.	1	–
source=<float>	Sets the source bias to apply. In general, it should be positive for NMOS devices and negative for PMOS devices.	0.0	V
substrate=<float>   <list>	Sets the substrate bias to apply as either a single value or a comma-separated list of values.  To reverse bias the substrate, the value must be negative for NMOS devices and positive for PMOS devices.	0.0	V

## Appendix B: Input File Commands

### contact Command

#### Examples

Specify multiple values for the drain bias:

```
bias drain=0.05,1.00
```

---

## contact Command

This command controls the contact parameters used by Garand and Garand MC (see [Specifying Contacts on page 77](#)).

#### Syntax

```
contact <parameter>=<value>
```

Parameter	Description	Default	Unit
<b>Parameters common to Garand and Garand MC</b>			
resistance_convergence_max=<float>	Sets the relative change in current from one iteration to the next <i>below which</i> contact potentials will be updated due to contact resistance.	$10^{-1}$	—
resistance_convergence_min=<float>	Sets the relative change in current from one iteration to the next <i>above which</i> contact potentials will be updated due to contact resistance.	$5 \times 10^{-4}$	—
resistance_lumped_drain=<float>	Sets the resistance for the drain contact only.	Value set by resistance_lumped	$\Omega$
resistance_lumped_source=<float>	Sets the resistance for the source contact only.	Value set by resistance_lumped	$\Omega$
resistance_lumped=<float>	Sets the per-contact resistance to be applied as a lumped resistance. You can specify <code>resistance_lumped_drain</code> and <code>resistance_lumped_source</code> independently.	0.0	$\Omega$
resistivity_lumped_drain=<float>	Sets the drain contact resistivity to be applied as a lumped resistance.	Value set by resistivity_lumped	$\Omega \cdot \text{cm}^2$

## Appendix B: Input File Commands

### contact Command

Parameter	Description	Default	Unit
resistivity_lumped_source=<float>	Sets the source contact resistivity to be applied as a lumped resistance.	Value set by resistivity_lumped	$\Omega \cdot \text{cm}^2$
resistivity_lumped=<float>	Sets the per-contact resistivity to be applied as a lumped resistance. You can specify resistivity_lumped_source and resistivity_lumped_drain independently.	0.0	$\Omega \cdot \text{cm}^2$

#### Parameters specific to Garand only

confined_boundary=off   on	Specifies whether to apply a confined boundary condition to contacts. Options are: <ul style="list-style-type: none"> <li>off: Do not apply a confined boundary condition to contacts.</li> <li>on: Apply a confined boundary condition to contacts.</li> </ul>	off	-
fill=<float>   max	Sets the doping level for source and drain contacts as either a defined value or the maximum value found in the contacts.	-	$\text{cm}^{-3}$
poly_shift=<float>	Sets the polysilicon gate ‘workfunction’ shift.	0.0	V
polyfill=<float>   max	Sets the doping level for polysilicon gate contacts as either a defined value or the maximum value found in the polysilicon gate contact.	-	$\text{cm}^{-3}$
resistance_damping=<float>	Sets the damping factor to use when updating contact potentials due to the updated calculation of the voltage drop across the external contact resistance.	0.25	-
resistivity_distrib_drain=<float>	Sets the drain contact resistivity to be applied as a distributed resistance.	Value set by resistivity_distrib	$\Omega \cdot \text{cm}^2$
resistivity_distrib_source=<float>	Sets the source contact resistivity to be applied as a distributed resistance.	Value set by resistivity_distrib	$\Omega \cdot \text{cm}^2$

## Appendix B: Input File Commands

### contact Command

Parameter	Description	Default	Unit
resistivity_distrib=<float>	Sets the per-contact resistivity to be applied as a distributed resistance. You can specify resistivity_distrib_source and resistivity_distrib_drain independently.	0.0	$\Omega \cdot \text{cm}^2$
sigma_resistance=<float>	Sets the standard deviation for contact resistance.	—	$\Omega$
sigma_resistivity=<float>	Sets the standard deviation for contact resistivity.	—	$\Omega \cdot \text{cm}^2$
void_fill= off   on	Specifies whether to include any void or gas regions connected to contacts as part of the contact metal. Options are: <ul style="list-style-type: none"> <li>off: Do not include any void or gas regions connected to contacts.</li> <li>on: Include any void or gas regions connected to contacts.</li> </ul>	off	—
wf_sigma=<float>	Sets the standard deviation for Gaussian workfunction variation.	—	eV
work_function=<float>	Sets the metal-gate workfunction.	4.0	eV

#### Parameters specific to Garand MC only

decouple_depth=<integer>	Sets the number of cells adjacent to an electrostatic contact to be decoupled (positive integer value).	0	—
decouple_diff=<float>	Sets the percentage to use (positive value).	0	%
decouple_drain= off   on	Specifies whether to decouple electrostatic drain contacts from MC transport automatically. Options are: <ul style="list-style-type: none"> <li>off: Do not decouple electrostatic drain contacts.</li> <li>on: Decouple electrostatic drain contacts.</li> </ul>	off	—
decouple_Emax=<float>	Sets the maximum field to use (positive value).	0	kV/cm

## Appendix B: Input File Commands

### contact Command

Parameter	Description	Default	Unit
decouple_offset= <float>	Sets the maximum separation to use (positive value).	0	nm
decouple_source= off   on	Specifies whether to decouple electrostatic source contacts from MC transport automatically. Options are: <ul style="list-style-type: none"><li>• off: Do not decouple electrostatic source contacts.</li><li>• on: Decouple electrostatic source contacts.</li></ul>	off	—
injection_dist= off   on	Specifies whether to evaluate the velocity-weighted injection distribution for use in defining injection states. Options are: <ul style="list-style-type: none"><li>• off: Do not evaluate the velocity-weighted injection distribution.</li><li>• on: Evaluate the velocity-weighted injection distribution.</li></ul>	off	—
resistance_current_min = <float>	Sets the minimum drain current to which contact resistance is applied.	1e-7	A
resistance_max_loops= <integer>	Sets the number of contact potential updates when contact resistance is applied.	20	—
resistance_tolerance= <float>	Sets the upper value of the percentage error in the current that must be achieved before the contact potential is updated due to the inclusion of contact resistance ( $0 < \text{resistance\_tolerance} \leq 100$ ).	5.0	%

---

## Defining Contacts

The input parameters for a contact definition require multiple values to be specified on one line (see [Specifying Contact Locations on page 78](#)).

**Note:**

This command applies only to Garand.

## Appendix B: Input File Commands

### contact Command

#### Syntax

```
contact <name> <parameter>=<value>
```

Parameter	Description	Default	Unit
<name>	Sets the type of contact to be defined. Options are: <ul style="list-style-type: none"><li>• drain: Drain contact</li><li>• fixed_gate: Fixed-gate contact</li><li>• metal_gate: Metal-gate contact</li><li>• ohmic: Generic Ohmic contact</li><li>• poly_gate: Poly-gate contact</li><li>• source: Source contact</li><li>• substrate: Substrate contact</li></ul>	—	—
barrier=<float>	Applies only to <code>fixed_gate</code> , <code>metal_gate</code> , and <code>poly_gate</code> . Sets the workfunction difference between a metal gate and the intrinsic reference semiconductor, or sets a Fermi-level offset in a polysilicon gate. You cannot specify a value for <code>work_function</code> in the <code>contact</code> command if <code>barrier</code> is specified.	—	eV
bias=<float>	Sets the bias (see <a href="#">Specifying the Bias on page 79</a> ).	—	V
filter=<string>	Sets the filter to be applied within the contact volume (see <a href="#">Specifying a Filter on page 79</a> ).	—	—
import=<string>	Sets the field in the TDR file that defines the points in the contact.	—	—
name=<string>	Sets the name of the contact that is used as the label to identify data saved in the database.	—	—
work_function=<float>	Applies only to <code>metal_gate</code> and <code>fixed_gate</code> . Sets the workfunction to use for the gate contact. You can specify <code>barrier</code> or <code>work_function</code> , but not both.	—	eV
xmax=<float>	Sets the contact maximum position in the x-direction. If not specified, the x-maximum of the device is assumed.	—	Input unit <sup>1</sup>
xmin=<float>	Sets the contact minimum position in the x-direction. If not specified, the x-minimum of the device is assumed.	—	Input unit <sup>1</sup>

## Appendix B: Input File Commands

### doping Command

Parameter	Description	Default	Unit
ymax=<float>	Sets the contact maximum position in the y-direction. If not specified, the y-maximum of the device is assumed.	—	Input unit <sup>1</sup>
ymin=<float>	Sets the contact minimum position in the y-direction. If not specified, the x-minimum of the device is assumed.	—	Input unit <sup>1</sup>
zmax=<float>	Sets the contact maximum position in the z-direction. If not specified, the z-maximum of the device is assumed.	—	Input unit <sup>1</sup>
zmin=<float>	Sets the contact minimum position in the z-direction. If not specified, the z-minimum of the device is assumed.	—	Input unit <sup>1</sup>

1. The default input unit for Garand is the nanometer, but it can be changed (see [Dimensional Unit on page 45](#)).

### Examples

Define the source contact:

```
contact source xmax=-15.0 ymin=-10.0 ymax=10.0 zmin=-5.0 zmax=0.0 \
filter=semiconductor
```

---

## doping Command

This command controls the doping parameters in Garand (see [Doping Profiles on page 63](#)).

#### Note:

All commands in this section apply only to Garand.

#### Syntax

```
doping <parameter>=<value>
```

Add or replace doping, with multiple options on one line (see [User-Added Doping on page 66](#)):

```
doping (add | replace) type=<string> field=<string> peak=<float> \
material=<string> region=<string> \
sigma-x=<float> sigma-y=<float> sigma-z=<float> \
xmin=<float> xmax=<float> ymin=<float> ymax=<float> \
zmin=<float> zmax=<float>
```

## Appendix B: Input File Commands

### doping Command

Parameter	Description	Default	Unit
max_doping=<float>	Sets the maximum doping concentration allowed in a structure.	$1 \times 10^{22}$	cm <sup>-3</sup>
<b>Parameters specific to adding or replacing doping</b>			
field=<string>	Sets a doping field to which the doping should be added. This can be an existing field (such as ArsenicActiveConcentration) or a new field.  The default is AddedAcceptorConcentration for acceptors and AddedDonorConcentration for donors.	See <a href="#">User-Added Doping on page 66</a>	—
material=<string>	Sets a material to which the added doping should be restricted.	—	—
peak=<float>	Sets the peak doping concentration to be added.	0.0	cm <sup>-3</sup>
region=<string>	Sets a region to which the added doping should be restricted.	—	—
sigma-x=<float>	Sets the standard deviation for a Gaussian roll-off of doping concentration in the x-direction outside of the specified bounding box.	0.0	nm
sigma-y=<float>	Sets the standard deviation for a Gaussian roll-off of doping concentration in the y-direction outside of the specified bounding box.	0.0	nm
sigma-z=<float>	Sets the standard deviation for a Gaussian roll-off of doping concentration in the z-direction outside of the specified bounding box.	0.0	nm
type=<string>	Sets the type of doping to be added. Options are: <ul style="list-style-type: none"><li>• acceptor: Add acceptor-type doping.</li><li>• donor: Add donor-type doping.</li></ul>	—	—
xmax=<float>	Sets the upper x-boundary of the peak doping region.	Maximum x-boundary	Input unit <sup>1</sup>

## Appendix B: Input File Commands

### mesh Command

Parameter	Description	Default	Unit
xmin=<float>	Sets the lower x-boundary of the peak doping region.	Minimum x-boundary	Input unit <sup>1</sup>
ymin=<float>	Sets the upper y-boundary of the peak doping region.	Maximum y-boundary	Input unit <sup>1</sup>
zmin=<float>	Sets the lower z-boundary of the peak doping region.	Minimum z-boundary	Input unit <sup>1</sup>
ymax=<float>	Sets the upper y-boundary of the peak doping region.	Maximum y-boundary	Input unit <sup>1</sup>
zmax=<float>	Sets the upper z-boundary of the peak doping region.	Maximum z-boundary	Input unit <sup>1</sup>

1. The default input unit for Garand is the nanometer, but it can be changed (see [Dimensional Unit on page 45](#)).

---

## mesh Command

This command imports the simulation mesh from a TDR file or specifies a simulation mesh directly in the input file.

### Note:

All commands in this section apply only to Garand.

### Syntax

Import a mesh from a TDR file (see [Importing a Mesh on page 52](#)):

```
mesh import [xmin=<float>] [xmax=<float>] \
            [ymin=<float>] [ymax=<float>] \
            [zmin=<float>] [zmax=<float>]
```

Specify a mesh (see [Specifying a Mesh on page 52](#)):

```
mesh x start=<float> end=<float> (spaces=<integer> | step=<integer>) \
      [first=<float>] [last=<float>]
mesh y start=<float> end=<float> (spaces=<integer> | step=<integer>) \
      [first=<float>] [last=<float>]
mesh z start=<float> end=<float> (spaces=<integer> | step=<integer>) \
      [first=<float>] [last=<float>]
```

## Appendix B: Input File Commands

### mesh Command

Specify a mesh using alternative method (see [Alternative Mesh Specification on page 55](#)):

```
mesh x pos=<float> dh=<float>
mesh y pos=<float> dh=<float>
mesh z pos=<float> dh=<float>
```

Parameter	Description	Default	Unit
<b>Importing a mesh</b>			
xmax=<float>	Sets the maximum value in the x-direction for the simulation domain.	–	Input unit <sup>1</sup>
xmin=<float>	Sets the minimum value in the x-direction for the simulation domain.	–	Input unit <sup>1</sup>
ymax=<float>	Sets the maximum value in the y-direction for the simulation domain.	–	Input unit <sup>1</sup>
ymin=<float>	Sets the minimum value in the y-direction for the simulation domain.	–	Input unit <sup>1</sup>
zmax=<float>	Sets the maximum value in the z-direction for the simulation domain.	–	Input unit <sup>1</sup>
zmin=<float>	Sets the minimum value in the z-direction for the simulation domain.	–	Input unit <sup>1</sup>
<b>Specifying a mesh</b>			
end=<float>	Sets the end point of the region.	–	Input unit <sup>1</sup>
first=<float>	Sets the specific length of the first mesh space in the region.	–	Input unit <sup>1</sup>
last=<float>	Sets the specific length of the last mesh space in the region.	–	Input unit <sup>1</sup>
spaces=<integer>	Sets the number of mesh spaces that should be in the region specified by start and end.	–	–
start=<float>	Sets the start point of the region.	–	Input unit <sup>1</sup>
step=<float>	Sets the step size. If you specify this parameter, then you cannot specify first or last.	–	Input unit <sup>1</sup>

## Appendix B: Input File Commands

### mesh Command

Parameter	Description	Default	Unit
<b>Specifying a mesh using alternative method</b>			
dh=<float>	Sets the mesh spacing on either side of the given position ( <i>pos</i> ).	—	Input unit <sup>1</sup>
pos=<float>	Sets the position of the key mesh points.	—	Input unit <sup>1</sup>

1. The default input unit for Garand is the nanometer, but it can be changed (see [Dimensional Unit on page 45](#)).

### Examples

Generate an  $80 \times 30 \times 160$  nm<sup>3</sup> simulation domain with 1-nm mesh spacing in each direction:

```
mesh x start=-40 end=40 spaces=80
mesh y start=0 end=30 spaces=30
mesh z start=-140 end=20 spaces=160
```

Then, overwrite the middle 30 nm in the x-direction with a 0.5-nm mesh spacing, for example, to resolve the MOSFET channel region:

```
mesh x start=-15 end=15 step=0.5
```

Replace the mesh from  $z = -140$  nm to 0 nm, with 25 mesh spaces in such a way that the last mesh space (at  $z = 0$ ) will be 1 nm:

```
mesh z start=-140 end=0 spaces=25 last=1
```

Use an alternative mesh specification based on specifying a series of mesh line positions (*pos*) with an associated mesh spacing (*dh*) applied to either side of this position:

```
mesh x pos=0 dh=10
mesh x pos=25 dh=0.5
mesh x pos=30 dh=0.5
mesh x pos=50 dh=5
```

## Appendix B: Input File Commands

### model Command

---

## model Command

This command specifies additional models to be included in Garand simulations (see [Additional Models on page 122](#)).

---

## Specifying Simple Models

You can specify simple models (see [Density-Gradient Quantum Corrections on page 122](#)).

**Note:**

All commands in this section apply only to Garand.

### Syntax

```
model <parameter>=<value>
```

Parameter	Description	Default	Unit
density_gradient=off   on	Specifies whether to use density-gradient quantum corrections in the simulation. Options are: <ul style="list-style-type: none"><li>• off: Do not use density-gradient quantum corrections.</li><li>• on: Use density-gradient quantum corrections.</li></ul>	off	—
dg_doping_limit=<float>	Sets a limit in the doping concentration above which density-gradient interface boundary conditions are not applied.	$1 \times 10^{20}$	$\text{cm}^{-3}$
dg_sdevice_bc=off   on	Specifies whether to use the default Sentaurus Device boundary conditions at oxide interfaces. Options are: <ul style="list-style-type: none"><li>• off: Do not use Sentaurus Device boundary conditions.</li><li>• on: Use Sentaurus Device boundary conditions.</li></ul>	off	—
eprp_method=<string>	Sets the directional component of the perpendicular electric field that is considered to be <i>perpendicular</i> . Options are: <ul style="list-style-type: none"><li>• normal_to_current: Normal to the direction of the current flow</li><li>• normal_to_interface: Normal to the nearest interface</li></ul>	normal_to_interface	—

## Appendix B: Input File Commands

### model Command

Parameter	Description	Default	Unit
minority_dg= off   on	Specifies whether to solve density-gradient quantum corrections for the minority carriers. Options are: <ul style="list-style-type: none"><li>• off: Do not solve density-gradient quantum corrections.</li><li>• on: Solve density-gradient quantum corrections.</li></ul>	off	—
minority_dg_bc= off   on	Specifies whether to apply density-gradient boundary conditions at insulator interfaces when solving the DG equation for minority carriers. Options are: <ul style="list-style-type: none"><li>• off: Do not apply DG boundary conditions.</li><li>• on: Apply DG boundary conditions.</li></ul>	on	—
poly_dg= off   on	Specifies whether to solve the density gradient equation within polysilicon gates. Options are: <ul style="list-style-type: none"><li>• off: Do not solve the DG equation.</li><li>• on: Solve the DG equation.</li></ul>	on	—
strainx_doping_limit=<float>	Sets the doping concentration below which the mobility is scaled by the factor strainx. See <a href="#">Low-Field Mobility Modifiers on page 321</a> .	$1 \times 10^{20}$	$\text{cm}^{-3}$

---

## Using Model Identifiers

Some models require multiple parameters, in which case, the model itself is identified with a specific model identifier of the form:

```
model <model_identifier> <parameter>=<value> ...
```

## Poisson–Schrödinger Quantum Corrections

For Poisson–Schrödinger quantum corrections, the model identifier is `schrödinger`. See [Schrödinger Quantum Corrections on page 125](#).

**Note:**

This command applies only to Garand.

### Syntax

```
model schrödinger <parameter>=<value>
```

## Appendix B: Input File Commands

### model Command

Parameter	Description	Default	Unit
status= off   on	Specifies whether to use the Schrödinger model. Options are: <ul style="list-style-type: none"><li>• off: Do not use the Schrödinger model.</li><li>• on: Use the Schrödinger model.</li></ul>	off	—
1d_confinement_direction=<string>	When confinement=1D, this parameter sets the confinement direction. Options are: <ul style="list-style-type: none"><li>• x: Confinement along the x-direction</li><li>• y: Confinement along the y-direction</li><li>• z: Confinement along the z-direction</li></ul>	—	—
confinement=<string>	Sets the number of confinement directions. Options are: <ul style="list-style-type: none"><li>• 1D: 1D confinement</li><li>• 2D: 2D confinement</li></ul>	2D	—
enable_complex_checks= off   on	Specifies whether to check for complex solutions of the Schrödinger equation (only checks the num_subbands applied). Options are: <ul style="list-style-type: none"><li>• off: Do not check for complex solutions.</li><li>• on: Check for complex solutions.</li></ul>	off	—
enable_dirichlet_boundary= off   on	Specifies whether to apply a Dirichlet boundary to the outer domain of the Schrödinger solution. Options are: <ul style="list-style-type: none"><li>• off: Do not apply a Dirichlet boundary.</li><li>• on: Apply a Dirichlet boundary.</li></ul>	on	—
enable_metal_bounds= off   on	Specifies whether to treat Air materials in the Poisson–Schrödinger solver as metals. Options are: <ul style="list-style-type: none"><li>• off: Do not treat Air materials as metals.</li><li>• on: Treat Air materials as metals.</li></ul>	off	—
max_iterations=<integer>	Sets the upper limit of iterations that must be completed by the Poisson–Schrödinger solver.	50	—
num_subbands=<integer>	Sets the number of subbands to be resolved within the Schrödinger solution.	20	—

## Appendix B: Input File Commands

### model Command

Parameter	Description	Default	Unit
potential_accuracy=<float>	Sets the convergence criterion for the Poisson–Schrödinger solver, based on the absolute error of the potential.	$10^{-3}$	—
splitting_point=<float>	Sets the position at which to extract valley-splitting information. It is always relative to the direction of transport.	0.0	—
xmax=<float>	Sets the solution domain maximum position in the x-direction. If not specified, the x-maximum of the device is assumed.	—	nm
xmin=<float>	Sets the solution domain minimum position in the x-direction. If not specified, the x-minimum of the device is assumed.	—	nm
ymax=<float>	Sets the solution domain maximum position in the y-direction. If not specified, the y-maximum of the device is assumed.	—	nm
ymin=<float>	Sets the solution domain minimum position in the y-direction. If not specified, the y-minimum of the device is assumed.	—	nm
zmax=<float>	Sets the solution domain maximum position in the z-direction. If not specified, the z-maximum of the device is assumed.	—	nm
zmin=<float>	Sets the solution domain minimum position in the z-direction. If not specified, the z-minimum of the device is assumed.	—	nm

## Schrödinger Boundary Conditions

You can select additional Schrödinger boundary conditions for arbitrary energy barriers (see [Adding Schrödinger Boundaries on page 129](#)).

### Note:

This command applies only to Garand.

### Syntax

```
model schrodinger boundary <parameter>=<value>
```

## Appendix B: Input File Commands

### model Command

Parameter	Description	Default	Unit
affinity=<float>	Sets the affinity level for the energy barrier.	–	eV
xmin=<float>	Sets the boundary minimum position in the x-direction. If not specified, the x-minimum of the device is assumed.	–	nm
xmax=<float>	Sets the boundary maximum position in the x-direction. If not specified, the x-maximum of the device is assumed.	–	nm
ymin=<float>	Sets the boundary minimum position in the y-direction. If not specified, the y-minimum of the device is assumed.	–	nm
ymax=<float>	Sets the boundary maximum position in the y-direction. If not specified, the y-maximum of the device is assumed.	–	nm
zmin=<float>	Sets the boundary minimum position in the z-direction. If not specified, the z-minimum of the device is assumed.	–	nm
zmax=<float>	Sets the boundary maximum position in the z-direction. If not specified, the z-maximum of the device is assumed.	–	nm

## Fermi–Dirac Statistics

Fermi–Dirac statistics can be activated by using the model identifier `fermi_dirac`.

### Note:

This command applies to Garand and Garand MC.

### Syntax

```
model fermi_dirac <parameter>=<value>
```

Parameter	Description	Default	Unit
status= off   on	Specifies whether to use Fermi–Dirac carrier statistics in the simulation. Options are: <ul style="list-style-type: none"><li>• off: Use Maxwell–Boltzmann statistics.</li><li>• on: Use Fermi–Dirac statistics.</li></ul>	off	–

## Appendix B: Input File Commands

### model Command

## Band-to-Band Tunneling Model

For the band-to-band tunneling model, the model identifier is `drain_leakage` (see [Drain Leakage on page 134](#)).

#### Note:

This command applies only to Garand.

#### Syntax

```
model drain_leakage <parameter>=<value>
```

Parameter	Description	Default	Unit
<code>status= off   on</code>	Specifies whether to use the band-to-band tunneling model in the simulation. Options are: <ul style="list-style-type: none"><li>• <code>off</code>: Do not use the band-to-band tunneling model.</li><li>• <code>on</code>: Use the band-to-band tunneling model.</li></ul>	<code>off</code>	—
<code>deltapot=&lt;float&gt;</code>	Applies only to <code>method=local</code> . Two times the potential by which the conduction band should vary in the direction of the electric field within a distance $\text{deltapot} \times (qE_g)/F$ in order that the generation term calculated at a mesh node should be used (see <a href="#">Specifying Fraction of Band Gap on page 137</a> ).	1.0	—
<code>kaneA=&lt;float&gt;</code>	Applies only to <code>method=local</code> . Sets the prefactor used in the Kane formula. It can be user specified if required for fitting experimental data.	—	$\text{cm}^{-3} \text{s}^{-1}$
<code>kaneB=&lt;float&gt;</code>	Applies only to <code>method=local</code> . Sets the factor used in the exponential of the Kane formula. It can be user specified if required for fitting experimental data.	—	V/cm
<code>kaneEg=&lt;float&gt;</code>	Applies only to <code>method=local</code> . Sets the band gap used in the prefactor and the exponential of the Kane formula. It can be user specified if required for fitting experimental data.	—	eV

## Appendix B: Input File Commands

### model Command

Parameter	Description	Default	Unit
kaneP=<float>	Applies only to method=local. Sets the power exponent used in the Kane formula: <ul style="list-style-type: none"><li>• Set kaneP=2.0 for direct tunneling.</li><li>• Set kaneP=2.5 for indirect tunneling.</li></ul>	2.0	—
method=<string>	Sets which model to use for the leakage calculation. Options are: <ul style="list-style-type: none"><li>• local: Use the Kane local band-to-band tunneling model (see <a href="#">Modified Kane Local Model on page 135</a>).</li><li>• nonlocal: Use the nonlocal band-to-band tunneling model (see <a href="#">Dynamically Adapted Nonlocal Model on page 137</a>).</li></ul>	local	—
min_dist=<float>	Applies only to method=local. Sets the minimum distance from the dielectric interfaces from which to start calculating band-to-band tunneling.	0.0	nm

## Shockley–Read–Hall Generation–Recombination

The identifier for the Shockley–Read–Hall (SRH) model is **srh** (see [Shockley–Read–Hall Generation–Recombination on page 140](#)).

### Note:

This command applies only to Garand.

### Syntax

```
model srh <parameter>=<value>
```

Parameter	Description	Default	Unit
status= off   on	Specifies whether to use the SRH model in the simulation. Options are: <ul style="list-style-type: none"><li>• off: Do not use the SRH model.</li><li>• on: Use the SRH model.</li></ul>	off	—
doping_dependence= off   on	Specifies whether to include doping dependence in the SRH model. Options are: <ul style="list-style-type: none"><li>• off: Do not include doping dependence.</li><li>• on: Include doping dependence.</li></ul>	off	—

## Appendix B: Input File Commands

### model Command

Parameter	Description	Default	Unit
tau_n=<float>	Sets the lifetime for electrons.	1e-5	s
tau_p=<float>	Sets the lifetime for holes.	3e-6	s
trap_energy=<float>	Sets $E_{\text{trap}}$ , which is the energy level of the traps relative to the mid-gap. Positive values are closer to the conduction band. Negative values are closer to the valence band.	0.0	eV

## User-Specified Trap Positions

You can add discrete trap positions in the SRH generation calculation (see [User-Specified Trap Positions on page 144](#)).

### Note:

This command applies only to Garand.

### Syntax

```
model srh_add_trap <parameter>=<value> <parameter1>=<value1> ...
```

Parameter	Description	Default	Unit
trap_energy=<float>	Sets the energy level of the traps relative to the mid-gap. Positive values are closer to the conduction band. Negative values are closer to the valence band.	0.0	eV
x=<float>	Sets the x-coordinate of the trap position.	0.0	Input unit <sup>1</sup>
xsec_n=<float>	Sets the trap cross-section for electrons.	1e-15	cm <sup>2</sup>
xsec_p=<float>	Sets the trap cross-section for holes.	1e-15	cm <sup>2</sup>
y=<float>	Sets the y-coordinate of the trap position.	0.0	Input unit <sup>1</sup>
z=<float>	Sets the z-coordinate of the trap position.	0.0	Input unit <sup>1</sup>

1. The default input unit for Garand is the nanometer, but it can be changed (see [Dimensional Unit on page 45](#)).

## Appendix B: Input File Commands

### model Command

## Random Trap Positions

You can include random SRH traps by using the identifier `random_srh_traps` (see [Random Trap Positions on page 145](#)).

**Note:**

This command applies only to Garand.

### Syntax

```
model random_srh_traps <parameter>=<value>
```

Parameter	Description	Default	Unit
<code>status= off   on</code>	Specifies whether to include random SRH traps in the simulation. Options are: <ul style="list-style-type: none"><li>• <code>off</code>: Do not include random SRH traps.</li><li>• <code>on</code>: Include random SRH traps.</li></ul>	<code>off</code>	—
<code>grid_resolution= &lt;float&gt;</code>	Specifies the resolution in all directions of the 3D grid of trap positions that will be looped over when <code>use_grid=on</code> .	1.0	nm
<code>grid_resolution_x= &lt;float&gt;</code>	Specifies the resolution in the x-direction of the 3D grid of trap positions that will be looped over when <code>use_grid=on</code> .	*1	nm
<code>grid_resolution_y= &lt;float&gt;</code>	Specifies the resolution in the y-direction of the 3D grid of trap positions that will be looped over when <code>use_grid=on</code> .	*1	nm
<code>grid_resolution_z= &lt;float&gt;</code>	Specifies the resolution in the z-direction of the 3D grid of trap positions that will be looped over when <code>use_grid=on</code> .	*1	nm
<code>num_config= &lt;integer&gt;</code>	Sets the total number of trap configurations to use.	1	—
<code>repeat_config= off   on</code>	Specifies whether to repeat the same sequence of trap configurations for each statistical device number. Options are: <ul style="list-style-type: none"><li>• <code>off</code>: Each statistical device number has a different sequence of trap configurations.</li><li>• <code>on</code>: Repeat the same sequence of trap configurations for each statistical device number.</li></ul>	<code>off</code>	—

## Appendix B: Input File Commands

### model Command

Parameter	Description	Default	Unit
single_trap= off   on	Specifies whether to place a single trap randomly. Options are: <ul style="list-style-type: none"> <li>off: The number of traps in each configuration is generated statistically based on the trap density.</li> <li>on: Place a single trap in a random position.</li> </ul>	off	—
start_config= <integer>	Sets the starting trap configuration number.	1	—
trap_density= <float>	Sets the density of traps if not using a single trap.	1e15	cm <sup>-3</sup>
trap_energy_sigma= <float>	Sets the standard deviation in the energy level of the traps. If specified, then the trap energy of each discrete trap will vary randomly from the nominal value (trap_energy) following a Gaussian distribution, with this value of standard deviation.	0	eV
trap_energy= <float>	Sets the energy level of the traps relative to the mid-gap. Positive values are closer to the conduction band. Negative values are closer to the valence band.	0.0	eV
use_grid= off   on	Rather than generating the sequence of single trap positions randomly, a regular grid can be used. For each valid point on that grid, a leakage calculation is performed considering a single trap at that point. Options are: <ul style="list-style-type: none"> <li>off: Generate the sequence of trap positions randomly.</li> <li>on: Use a regular grid for the sequence of trap positions.</li> </ul>	off	—
xmax=<float>	Sets the maximum extent of the bounding box in the x-direction.	Maximum x-boundary	Input unit <sup>2</sup>
xmin=<float>	Sets the minimum extent of the bounding box in the x-direction.	Minimum x-boundary	Input unit <sup>2</sup>

## Appendix B: Input File Commands

### model Command

Parameter	Description	Default	Unit
xsec_n_sigma=<float>	Sets the standard deviation in the trap cross-section for electrons. If specified, then the trap cross-section of each discrete trap will vary randomly from the nominal value ( <code>xsec_n</code> ) following a log Gaussian distribution, with this value of standard deviation.	0	decade
xsec_n=<float>	Sets the trap cross-section for electrons.	1e-15	cm <sup>2</sup>
xsec_p_sigma=<float>	Sets the standard deviation in the trap cross-section for holes. If specified, then the trap cross-section of each discrete trap will vary randomly from the nominal value ( <code>xsec_p</code> ) following a log Gaussian distribution, with this value of standard deviation.	0	decade
xsec_p=<float>	Sets the trap cross-section for holes.	1e-15	cm <sup>2</sup>
ymin=<float>	Sets the maximum extent of the bounding box in the y-direction.	Maximum y-boundary	Input unit <sup>2</sup>
ymax=<float>	Sets the minimum extent of the bounding box in the y-direction.	Minimum y-boundary	Input unit <sup>2</sup>
zmin=<float>	Sets the maximum extent of the bounding box in the z-direction.	Maximum z-boundary	Input unit <sup>2</sup>
zmax=<float>	Sets the minimum extent of the bounding box in the z-direction.	Minimum z-boundary	Input unit <sup>2</sup>

1. The default value for `grid_resolution_x`, `grid_resolution_y`, and `grid_resolution_z` is the value specified by `grid_resolution` or its default value if `grid_resolution` is not specified.
2. The default input unit for Garand is the nanometer, but it can be changed (see [Dimensional Unit on page 45](#)).

## Trap-Assisted Tunneling for Shockley–Read–Hall Model

You can activate trap-assisted tunneling (TAT) for the SRH model by using the identifier `tat_leakage` (see [Trap-Assisted Tunneling on page 141](#)).

### Note:

This command applies only to Garand.

### Syntax

```
model tat_leakage <parameter>=<value>
```

## Appendix B: Input File Commands

### model Command

Parameter	Description	Default	Unit
status= off   on	Specifies whether to include TAT for the SRH model in the simulation. Options are: <ul style="list-style-type: none"><li>• off: Do not include TAT for the SRH model.</li><li>• on: Include TAT for the SRH model.</li></ul>	off	—
method=<string>	Sets which method to use for the TAT calculation. Options are: <ul style="list-style-type: none"><li>• local: Use the local Hurkx model (see <a href="#">Local Trap-Assisted Tunneling Model on page 142</a>).</li><li>• nonlocal: Use the nonlocal WKB model (see <a href="#">Nonlocal Trap-Assisted Tunneling Model on page 143</a>).</li></ul>	local	—
tunnel_mass_n=<float>	Sets the tunneling mass for electrons.	0.5	—
tunnel_mass_p=<float>	Sets the tunneling mass for holes.	0.5	—
<b>Parameter specific to local TAT model</b>			
max_field=<float>	Sets the maximum electric field to use in the local TAT model ( <code>method=local</code> ).	5e6	V/cm
<b>Parameter specific to nonlocal TAT model</b>			
radius=<float>	Sets the maximum distance from a discrete trap to which nonlocal tunneling is calculated ( <code>method=nonlocal</code> ).	10.0	nm

## Gate Leakage Model

The identifier for the gate leakage model is `gate_leakage` (see [Gate Leakage on page 148](#)).

### Note:

This command applies only to Garand.

### Syntax

```
model gate_leakage <parameter>=<value>
```

## Appendix B: Input File Commands

### model Command

Parameter	Description	Default	Unit
status= off   on	Specifies whether to use the gate tunneling model. Options are: <ul style="list-style-type: none"><li>• off: Do not use the gate tunneling model.</li><li>• on: Use the gate tunneling model.</li></ul>	off	—
mtunnel_chan=<float>	Sets the tunneling effective mass in the channel material.	0.90	—
mtunnel_gate=<float>	Sets the tunneling effective mass in the gate electrode material.	0.90	—
mtunnel_ox=<float>	Sets the tunneling effective mass in the gate dielectric.	0.48	—
tat_density=<float>	For trap-assisted tunneling, sets the sheet density of traps in the gate dielectric.	1e11	cm <sup>-2</sup>
tat_nu0=<float>	For trap-assisted tunneling, sets the attempt-to-escape frequency from the trap.	1e12	Hz
tat_xsection=<float>	For trap-assisted tunneling, sets the trap capture cross-section.	1e-14	cm <sup>2</sup>

## Interface Charge Model

The identifier for the interface charge model is `interface_charge` (see [Interface Charge on page 150](#)).

### Note:

This command applies only to Garand.

### Syntax

```
model interface_charge <parameter>=<value>
```

Parameter	Description	Default	Unit
status= off   on	Specifies whether to include the interface charge in the simulation. Options are: <ul style="list-style-type: none"><li>• off: Do not include the interface charge.</li><li>• on: Include the interface charge.</li></ul>	off	—
file=<string>	Sets the name of the file containing the distributions of traps within the band gap of the material specified.	—	—

## Appendix B: Input File Commands

### model Command

Parameter	Description	Default	Unit
material=<string>	Sets the material that will have the interface charge at its interfaces with insulators.	–	–

## Variation in Random Dopant Mobility

You can specify variation in random dopant mobility (see [Random Dopant Mobility Variation on page 159](#)).

### Note:

It is not necessary to specify all bounding box limits (`xmin`, `xmax`, and so on) as they will default to the maximum extent of the simulation domain in that direction.

This command applies only to Garand.

### Syntax

```
model rdd_mobility <parameter>=<value>
```

Parameter	Description	Default	Unit
status= off   on	Specifies whether to include RDD mobility variation in the simulation. Options are: <ul style="list-style-type: none"><li>• off: Do not include RDD mobility.</li><li>• on: Include RDD mobility.</li></ul>	off	–
xmin=<float>	Sets the lower x-boundary of the RDD mobility region.	Minimum x-boundary	Input unit <sup>1</sup>
xmax=<float>	Sets the upper x-boundary of the RDD mobility region.	Maximum x-boundary	Input unit <sup>1</sup>
ymin=<float>	Sets the lower y-boundary of the RDD mobility region.	Minimum y-boundary	Input unit <sup>1</sup>
ymax=<float>	Sets the upper y-boundary of the RDD mobility region.	Maximum y-boundary	Input unit <sup>1</sup>
zmin=<float>	Sets the lower z-boundary of the RDD mobility region.	Minimum z-boundary	Input unit <sup>1</sup>
zmax=<float>	Sets the upper z-boundary of the RDD mobility region.	Maximum z-boundary	Input unit <sup>1</sup>

1. The default input unit for Garand is the nanometer, but it can be changed (see [Dimensional Unit on page 45](#)).

## Appendix B: Input File Commands

### output Command

## output Command

This command specifies the simulation output for Garand and Garand MC (see [Output on page 166](#) and [Chapter 6 on page 237](#)).

### Syntax

```
output <parameter>=<value>
```

Parameter	Description	Default	Unit
<b>Parameters common to Garand and Garand MC</b>			
bands= off   on	Specifies whether to include the conduction and valence bands in the TDR file. Options are: <ul style="list-style-type: none"><li>• off: No bands output.</li><li>• on: Include bands output.</li></ul>	on	—
fermi= off   on	Specifies whether to include the quasi-Fermi level in the TDR file. Options are: <ul style="list-style-type: none"><li>• off: No quasi-Fermi level output.</li><li>• on: Include quasi-Fermi level output.</li></ul>	on	—
hierarchical= off   on	Specifies whether to generate an output hierarchy, including a <code>bias</code> directory. Options are: <ul style="list-style-type: none"><li>• off: No output hierarchy.</li><li>• on: Generate output hierarchy.</li></ul>	on	—
integral_charge= off   on	Specifies whether to extract the integrated charge density. Options are: <ul style="list-style-type: none"><li>• off: Do not extract the integrated charge density.</li><li>• on: Extract the integrated charge density.</li></ul>	off	—
integration_xmax= <float>	Sets the maximum value in the x-direction to limit the integration or averaging range.	—	Input unit <sup>1</sup>
integration_xmin= <float>	Sets the minimum value in the x-direction to limit the integration or averaging range.	—	Input unit <sup>1</sup>
integration_ymax= <float>	Sets the maximum value in the y-direction to limit the integration or averaging range.	—	Input unit <sup>1</sup>

## Appendix B: Input File Commands

### output Command

Parameter	Description	Default	Unit
integration_ymin= <float>	Sets the minimum value in the y-direction to limit the integration or averaging range.	–	Input unit <sup>1</sup>
integration_zmax= <float>	Sets the maximum value in the z-direction to limit the integration or averaging range.	–	Input unit <sup>1</sup>
integration_zmin= <float>	Sets the minimum value in the z-direction to limit the integration or averaging range.	–	Input unit <sup>1</sup>
weighted_velocity= off   on	Specifies whether to extract the weighted average velocity. Options are: <ul style="list-style-type: none"> <li>• off: Do not extract the weighted average velocity.</li> <li>• on: Extract the weighted average velocity.</li> </ul>	off	–

#### Parameters specific to Garand only

affinity= off   on	Specifies whether to include the electron affinity in the TDR file. Options are: <ul style="list-style-type: none"> <li>• off: No electron affinity output.</li> <li>• on: Include electron affinity output.</li> </ul>	on	–
autocutlines= off   on	Specifies whether to output autocutlines automatically when using the autoslice option. Options are: <ul style="list-style-type: none"> <li>• off: Do not output autocutlines.</li> <li>• on: Output autocutlines.</li> </ul>	on	–
automesh= off   on	Specifies whether to write the intermediate mesh file, generated by the automesh feature, in the current working directory. Options are: <ul style="list-style-type: none"> <li>• off: No intermediate mesh file.</li> <li>• on: Write intermediate mesh file.</li> </ul>	off	–
bandgap= off   on	Specifies whether to include the band gap in the TDR file. Options are: <ul style="list-style-type: none"> <li>• off: No bandgap output.</li> <li>• on: Include bandgap output.</li> </ul>	on	–
csv= off   on	Specifies whether to generate CSV output for plotting in Sentaurus Visual. Options are: <ul style="list-style-type: none"> <li>• off: No CSV output.</li> <li>• on: Generate CSV output.</li> </ul>	off	–

## Appendix B: Input File Commands

### output Command

Parameter	Description	Default	Unit
dat= off   on	Specifies whether to write I–V and C–V data to .dat files. Options are: <ul style="list-style-type: none"><li>• off: Do not write .dat output files.</li><li>• on: Write .dat output files.</li></ul>	on	—
dg_mass= off   on	Specifies whether to include the density-gradient calibration parameter in the TDR file. Options are: <ul style="list-style-type: none"><li>• off: Do not include calibration parameter.</li><li>• on: Include calibration parameter.</li></ul>	on	—
directory=<string>	Sets the path to the results file.	'results'	—
dos= off   on	Specifies whether to include the densities-of-states, $N_C$ and $N_V$ , in the TDR file. Options are: <ul style="list-style-type: none"><li>• off: No densities-of-states output.</li><li>• on: Include densities-of-states output.</li></ul>	on	—
experiment=<string>	Sets the header for the simulation results file.	'sim'	—
hierarchical_kvps= off   on	Specifies whether to use the hierarchical mode when saving keyword–value pairs to the database. Options are: <ul style="list-style-type: none"><li>• off: Do not use the hierarchical mode.</li><li>• on: Use the hierarchical mode.</li></ul>	off	—
lateral_autocutline_pos=<float>	Sets the position of the lateral cutline.	—	Input unit <sup>1</sup>
ler= off   on	Specifies whether to output line edge roughness (LER) to a file. Options are: <ul style="list-style-type: none"><li>• off: No LER output.</li><li>• on: Generate LER output.</li></ul>	off	—
log= off   on	Specifies whether to write information, warning, and error messages to a log file. Options are: <ul style="list-style-type: none"><li>• off: Do not write such messages to a log file.</li><li>• on: Write such messages to a log file.</li></ul>	on	—

## Appendix B: Input File Commands

### output Command

Parameter	Description	Default	Unit
mat_model= off   on	Specifies whether to write material parameter values used in the simulation to a material model file in the output directory. Options are: <ul style="list-style-type: none"><li>• off: Do not write material model file.</li><li>• on: Write material model file.</li></ul>	on	—
mc_transfer= off   on	Specifies whether to generate Monte Carlo transfer (MCT) file output for use with Garand MC. Options are: <ul style="list-style-type: none"><li>• off: No MCT file output.</li><li>• on: Generate MCT file output.</li></ul>	off	—
mesh= off   on	Specifies whether to output the mesh for each direction. Options are: <ul style="list-style-type: none"><li>• off: Do not output mesh.</li><li>• on: Output mesh.</li></ul> When you specify mesh=on, three files are written: <ul style="list-style-type: none"><li>• mesh-x.dat</li><li>• mesh-y.dat</li><li>• mesh-z.dat</li></ul> These files contain the mesh coordinates (in $\mu\text{m}$ , unless output units have been changed) in the respective x-, y-, and z-directions.	off	—
mobility= off   on	Specifies whether to include mobility output in the TDR file. Options are: <ul style="list-style-type: none"><li>• off: No mobility output.</li><li>• on: Include mobility output.</li></ul>	on	—
plt= off   on	Specifies whether to write I-V and C-V data to .plt files. Options are: <ul style="list-style-type: none"><li>• off: Do not write .plt output files.</li><li>• on: Write .plt output files.</li></ul>	on	—
tdr= off   on	Specifies whether to generate TDR output for visualization in Sentaurs Visual. Options are: <ul style="list-style-type: none"><li>• off: No TDR output.</li><li>• on: Generate TDR output.</li></ul>	off	—

## Appendix B: Input File Commands

### output Command

Parameter	Description	Default	Unit
units=<string>	Sets the unit for simulation output only. Options are: <ul style="list-style-type: none"><li>• nm</li><li>• um</li><li>• mm</li><li>• cm</li><li>• m</li></ul> This parameter overrides any unit set with the <code>units</code> parameter of the <code>structure</code> command (see <a href="#">structure Command on page 899</a> ).	um	—
user_materials= off   on	Specifies whether to write an abridged default material parameter file for use with the <code>--user-materials</code> command-line option. Options are: <ul style="list-style-type: none"><li>• off: Do not write a material parameter file.</li><li>• on: Write a material parameter file.</li></ul>	off	—
vertical_ autocutline_pos= <float>	Sets the position of the vertical cutline.	—	Input unit <sup>1</sup>
weighted_mobility= off   on	Specifies whether to extract the weighted average mobility. Options are: <ul style="list-style-type: none"><li>• off: Do not extract the weighted average mobility.</li><li>• on: Extract the weighted average mobility.</li></ul>	off	—

#### Parameters specific to Garand MC only

ballisticity= off   on	Specifies whether to gather statistics for the ensemble traveling source to drain and drain to source, so as to estimate ballisticity. Options are: <ul style="list-style-type: none"><li>• off: Do not gather statistics (no ballistic output).</li><li>• on: Gather statistics (include ballistic output).</li></ul>	off	—
band_dispersion= off   on	Specifies whether to write $E(k)$ dispersions to .plt files. Options are: <ul style="list-style-type: none"><li>• off: Do not write dispersions to files.</li><li>• on: Write dispersions to files.</li></ul>	off	—

## Appendix B: Input File Commands

### output Command

Parameter	Description	Default	Unit
discrete_scattering = off   on	Specifies whether to report the distribution of individual mechanisms, rather than an aggregate. See <a href="#">Scattering Distribution on page 245</a> . Options are: <ul style="list-style-type: none"> <li>off: Do not report the distribution of individual mechanisms.</li> <li>on: Report an aggregate of mechanisms.</li> </ul>	off	–
domain= off   on	Specifies whether to output the initial simulation domain. Options are: <ul style="list-style-type: none"> <li>off: Do not output the initial simulation domain.</li> <li>on: Output initial simulation domain.</li> </ul>	off	–
E_distribution= off   on	Specifies whether to output the average carrier energy distribution to file. Options are: <ul style="list-style-type: none"> <li>off: Do not write distribution to file.</li> <li>on: Write distribution to file.</li> </ul>	off	–
k_distribution= off   on	Specifies whether to output the average carrier wavevector distribution to file. Options are: <ul style="list-style-type: none"> <li>off: Do not write distribution to file.</li> <li>on: Write distribution to file.</li> </ul>	off	–
k_vec_kp_disp= <float>	Sets the scaling factor for the output of $E(k)$ dispersions.	0.5	$2\pi/a$
max_E_el=<float>	Sets the maximum energy for electron distributions.	–	eV
max_E_ho=<float>	Sets the maximum energy for hole distributions.	–	eV
MC_results= off   on	Specifies whether to write a TDR file for visualization. See <a href="#">Carrier Distributions on page 235</a> . Options are: <ul style="list-style-type: none"> <li>off: Do not write a TDR file.</li> <li>on: Write a TDR file.</li> </ul>	off	–

## Appendix B: Input File Commands

### output Command

Parameter	Description	Default	Unit
MC_results_all= off   on	Specifies whether to write a TDR file for visualization after each update to the contact potential. Options are: <ul style="list-style-type: none"><li>• off: Do not write TDR files after each potential update.</li><li>• on: Write a TDR file after each potential update.</li></ul>	off	—
mixed_mesh_tdr= <string>	Specifies the path to the TDR file of the mixed-element mesh. See <a href="#">Output to Mixed Mesh on page 235</a> .	—	—
N_dist_el=<integer>	Sets the number of bins for electron distributions.	—	—
N_dist_ho=<integer>	Sets the number of bins for hole distributions.	—	—
scattering_count= off   on	Specifies whether to output the distribution of all scattering events, both inelastic and elastic. See <a href="#">Scattering Distribution on page 245</a> . Options are: <ul style="list-style-type: none"><li>• off: Do not output distribution of all scattering events.</li><li>• on: Output distribution of all scattering events.</li></ul>	off	—
scattering_mesh= off   on	Specifies whether to record scattering events on the simulation mesh and write them to a file for visualization. See <a href="#">Scattering Distribution on page 245</a> . Options are: <ul style="list-style-type: none"><li>• off: Do not write scattering events to file.</li><li>• on: Write scattering events to file</li></ul>	off	—
scattering_rates= off   on	Specifies whether to write Monte Carlo scattering rates to file. Options are: <ul style="list-style-type: none"><li>• off: Do not write rates to file.</li><li>• on: Write rates to file.</li></ul>	off	—
separate_bands= off   on	Specifies whether to write carrier properties for each band and valley. Options are: <ul style="list-style-type: none"><li>• off: Do not separate statistics based on valley.</li><li>• on: Write carrier averages based on valley occupation.</li></ul>	off	—

## Appendix B: Input File Commands

### output Command

Parameter	Description	Default	Unit
stream_trajectories = off   on	Specifies whether to write the trajectories of all carriers associated with all streaming groups to a TDR file. See <a href="#">Carrier Trajectories in Streaming Group on page 235</a> . Options are: <ul style="list-style-type: none"><li>• off: Do not write carrier trajectories to a TDR file.</li><li>• on: Write carrier trajectories to a TDR file.</li></ul>	off	—
stream_trajectory_fields=<list>	Specifies a list of available fields to sample, limited to energy and potential. By default, the propagation time is mapped to the particle trajectories. See <a href="#">Carrier Trajectories in Streaming Group on page 235</a> .	—	—
time_evolution= off   on	Specifies whether to write the time evolution of carrier properties to screen and file. Options are: <ul style="list-style-type: none"><li>• off: Do not write time evolution of properties.</li><li>• on: Write time evolution of properties.</li></ul>	off	—
update_tdr= off   on	Specifies whether to update the TDR file at every intermittent step after the transient. Options are: <ul style="list-style-type: none"><li>• off: Do not update the TDR file.</li><li>• on: Update the TDR file.</li></ul>	off	—

1. The default input unit for Garand is the nanometer, but it can be changed (see [Dimensional Unit on page 45](#)).

---

## Exporting 1D Cutline Data

You can export 1D cutline data from an arbitrary line through the simulation domain (see [Exporting 1D Cutline Data on page 170](#)).

**Note:**

This command applies only to Garand.

### Syntax

```
output cutline <x1>=<d1> <x2>=<d2> data=<string> file=<string>
```

## Appendix B: Input File Commands

### output Command

Here, <x1> and <x2> are any two of x, y, and z. You must choose two directions that are normal to the direction of the cutline.

Parameter	Description	Default	Unit
x   y   z=<d1>	Sets the position of the cutline in the specified direction.	–	Input unit <sup>1</sup>
x   y   z=<d2>	Sets the position of the cutline in the specified direction.	–	Input unit <sup>1</sup>
data=<string>	Sets the quantity to be output along the cutline. Options are: <ul style="list-style-type: none"><li>• ConductionBandEnergy: Conduction band edge in eV</li><li>• ValenceBandEnergy: Valence band edge in eV</li><li>• eDensity: Electron concentration in cm<sup>-3</sup></li><li>• hDensity: Hole concentration in cm<sup>-3</sup></li><li>• ElectrostaticPotential: Electrostatic potential in V</li><li>• AcceptorConcentration: Acceptor concentration in cm<sup>-3</sup></li><li>• DonorConcentration: Donor concentration in cm<sup>-3</sup></li><li>• DopingConcentration: Net doping concentration, that is, abs(<math>N_A - N_D</math>) in cm<sup>-3</sup></li><li>• AcceptorConcentrationRDD: Effective acceptor concentration in cm<sup>-3</sup> after random discrete doping has been assigned</li><li>• DonorConcentrationRDD: Effective donor concentration in cm<sup>-3</sup> after random discrete doping has been assigned</li><li>• Mobility: Majority carrier mobility in the channel direction in cm<sup>2</sup>V<sup>-1</sup>s<sup>-1</sup> (mobility in a specific direction can be obtained by specifying Mobility-x, Mobility-y, or Mobility-z)</li><li>• QuasiFermiEnergy: Quasi-Fermi energy in eV</li><li>• VacuumEnergy: Vacuum level in eV</li></ul>	–	–

## Appendix B: Input File Commands

### reliability Command

Parameter	Description	Default	Unit
file=<string>	<p>Sets the name of the file in which to export the cutline data.</p> <p>You can include placeholders in the file name that are replaced with the relevant values specific to the simulation being run. Available placeholders are:</p> <ul style="list-style-type: none"><li>• %EXPT% is replaced with the experiment name set with the output experiment=&lt;string&gt; command.</li><li>• %VD% is replaced with the drain bias at which the cutline was obtained.</li><li>• %VC% is replaced with the gate bias at which the cutline was obtained.</li><li>• %VSUB% is replaced with the substrate bias at which the cutline was obtained.</li></ul> <p><b>Note:</b> These placeholders are case sensitive and must be capitalized exactly as shown.</p>	–	–

1. *The default input unit for Garand is the nanometer, but it can be changed (see Dimensional Unit on page 45).*

---

## reliability Command

This command adds discrete fixed charges associated with device degradation in Garand simulations (see [User-Specified Fixed Charge on page 119](#)). First, you can specify explicitly the location of trapped charges.

**Note:**

All commands in this section apply only to Garand.

### Syntax

```
reliability add <parameter>=<value>
```

Parameter	Description	Default	Unit
charge=<string>	Sets which trapped charge is defined. Options are: <ul style="list-style-type: none"><li>• acceptor: Add a single negative charge.</li><li>• donor: Add a single positive charge.</li><li>• &lt;float&gt;: Add a fixed amount of negative or positive charge.</li></ul>	–	–
x=<float>	Sets the x-position of the charge in the defined input units.	–	Input unit <sup>1</sup>

## Appendix B: Input File Commands

### reliability Command

Parameter	Description	Default	Unit
y=<float>	Sets the y-position of the charge in the defined input units.	–	Input unit <sup>1</sup>
z=<float>	Sets the z-position of the charge in the defined input units.	–	Input unit <sup>1</sup>

1. The default input unit for Garand is the nanometer, but it can be changed (see Dimensional Unit on page 45).

---

## Generating Positions of Interface-Trapped Charges

In addition, Garand can automatically generate the positions of interface-trapped charges (ITC) statistically based on a nominal sheet density (see [Interface-Trapped Charges on page 119](#)).

### Note:

Multiple `reliability ITC` commands are allowed to specify multiple insulator materials or different bounding regions.

### Syntax

```
reliability ITC <parameter>=<value>
```

Parameter	Description	Default	Unit
status= off   on	Specifies whether to include ITC in the simulation. Options are: <ul style="list-style-type: none"><li>• off: Do not include ITC.</li><li>• on: Include ITC.</li></ul>	off	–
density=<float>	Sets the sheet density for the trapped charges.	$1 \times 10^{11}$	$\text{cm}^{-2}$
material=<string>	Sets the oxide material at whose interface the traps should be placed.	–	–
xmin=<float>	Sets the lower x-boundary of the ITC region for imported structures.	Minimum x-boundary	Input unit <sup>1</sup>
xmax=<float>	Sets the upper x-boundary of the ITC region for imported structures.	Maximum x-boundary	Input unit <sup>1</sup>
ymin=<float>	Sets the lower y-boundary of the ITC region for imported structures.	Minimum y-boundary	Input unit <sup>1</sup>

## Appendix B: Input File Commands

### simulation Command

Parameter	Description	Default	Unit
ymax=<float>	Sets the upper y-boundary of the ITC region for imported structures.	Maximum y-boundary	Input unit <sup>1</sup>
zmin=<float>	Sets the lower z-boundary of the ITC region for imported structures.	Minimum z-boundary	Input unit <sup>1</sup>
zmax=<float>	Sets the upper z-boundary of the ITC region for imported structures.	Maximum z-boundary	Input unit <sup>1</sup>

1. The default input unit for Garand is the nanometer, but it can be changed (see [Dimensional Unit on page 45](#)).

## simulation Command

This command specifies the simulation setup (see [Input File Options on page 164](#) and [Output on page 166](#)).

### Syntax

```
simulation <parameter>=<value>
```

Parameter	Description	Default	Unit
<b>Parameters common to Garand and Garand MC</b>			
autoslice= off   on	Specifies whether to run an autoslice simulation. Options are: <ul style="list-style-type: none"><li>• off: Do not run an autoslice simulation.</li><li>• on: Run an autoslice simulation.</li></ul>	off	—
pos_dep= off   on	Specifies whether to calculate parameters based on the spatially varying mole fraction field (see <a href="#">Setting Region-Specific Material Parameters on page 61</a> ). Options are: <ul style="list-style-type: none"><li>• off: Do not calculate parameters based on the spatially varying mole fraction field.</li><li>• on: Calculate parameters based on the spatially varying mole fraction field.</li></ul>	on	—
T=<float>	Sets the ambient temperature to use in the simulation.	300	K
threads=<integer>	Sets the number of parallel threads to use (see <a href="#">Parallel Execution on page 41</a> ).	—	—

## Appendix B: Input File Commands

### simulation Command

Parameter	Description	Default	Unit
<b>Parameters specific to Garand only</b>			
accept_unconverged = off   on	Specifies whether to accept the result even if the solution has not converged. Options are: <ul style="list-style-type: none"> <li>• off: Do not accept the result.</li> <li>• on: Accept the result.</li> </ul>	off	—
autoslice_position =<string>	Sets how the autoslice position is defined. Options are: <ul style="list-style-type: none"> <li>• gate_mean: Use the mean channel-direction coordinate of every mesh point within the gate.</li> <li>• gate_middle: Use the midpoint of the gate in the channel direction.</li> <li>• &lt;position&gt;: Specify a position in the channel direction.</li> </ul>	gate_middle	—
bounded_fermi= off   on	Typically, the quasi-Fermi level should not extend outside of the range of the applied bias. This parameter specifies whether to force the Fermi level to be hard bounded by the applied bias, which can help to stabilize some simulations. Options are: <ul style="list-style-type: none"> <li>• off: Fermi level is not bounded.</li> <li>• on: Fermi level is bounded.</li> </ul>	off	—
cap_dv_bulk= <float>	Sets the capacitance calculation: change in bias applied to the bulk or substrate contact when calculating the capacitive response to that contact.	0.05	V
cap_dv_drain= <float>	Sets the capacitance calculation: change in bias applied to the drain contact when calculating the capacitive response to that contact.	0.01	V
cap_dv_gate= <float>	Sets the capacitance calculation: change in bias applied to the gate contact when calculating the capacitive response to that contact.	0.01	V

## Appendix B: Input File Commands

### simulation Command

Parameter	Description	Default	Unit
cap_dv_source= <float>	Sets the capacitance calculation: change in bias applied to the source contact when calculating the capacitive response to that contact.	0.01	V
capacitance= <string>	Sets which capacitances to calculate. Options are: <ul style="list-style-type: none"><li>• all: Calculate the full capacitance matrix with the response to each of the four contacts.</li><li>• bulk: Calculate the capacitance response to the bulk contact, that is, <math>C_{gb}</math>, <math>C_{sb}</math>, <math>C_{db}</math>, and <math>C_{bb}</math>.</li><li>• drain: Calculate the capacitance response to the drain contact, that is, <math>C_{gd}</math>, <math>C_{sd}</math>, <math>C_{dd}</math>, and <math>C_{bd}</math>.</li><li>• gate: Calculate the capacitance response to the gate contact, that is, <math>C_{gg}</math>, <math>C_{sg}</math>, <math>C_{dg}</math>, and <math>C_{bg}</math>.</li><li>• off: Do not calculate capacitances.</li><li>• on: Calculate the full capacitance matrix with the response to each of the four contacts.</li><li>• source: Calculate the capacitance response to the source contact, that is, <math>C_{gs}</math>, <math>C_{ss}</math>, <math>C_{ds}</math>, and <math>C_{bs}</math>.</li></ul>	off	—
cce_solver= <string>	Sets the solver to use to solve the current continuity equation. Options are: <ul style="list-style-type: none"><li>• BiCGSTAB: Use the Bi-CGSTAB solver.</li><li>• BiCGSTAB2: Use the Bi-CGSTAB2 solver.</li></ul>	BiCGSTAB2	—
current_integration= <integer>	Sets the current integration method to use (see <a href="#">Alternative Current Integration Method on page 164</a> ). Options are: <ul style="list-style-type: none"><li>• 1: Selects the original method.</li><li>• 2: Selects the alternative method.</li></ul>	2	—
density_limit= <float>	Sets the maximum carrier density permitted in the structure during the simulation.	$1 \times 10^{22}$	cm <sup>-3</sup>
dg_start_iter= <integer>	Sets the Gummel iteration at which the solution of the density gradient equation should start to be included.	1	—

## Appendix B: Input File Commands

### simulation Command

Parameter	Description	Default	Unit
enforce_serial_for_mct= off   on	Specifies whether a Garand simulation that should produce an MCT file is forced to run single-threaded. Options are: <ul style="list-style-type: none"> <li>off: Allow parallel execution.</li> <li>on: Enforce serial execution.</li> </ul>	on	—
epscurr=<float>	Sets the tolerance to which the current continuity equation must be solved.	1e-7	—
epsdg=<float>	Sets the tolerance to which the density gradient equation must be solved.	1e-5	—
espois=<float>	Sets the tolerance to which the Poisson equation must be solved.	1e-5	—
fail_on_unconverged= off   on	Specifies whether the simulation should stop and fail immediately if it fails to converge for an I–V point. Options are: <ul style="list-style-type: none"> <li>off: If an I–V point fails to converge, then the simulation continues to simulate further I–V points.</li> <li>on: If an I–V point fails to converge, then the simulation stops immediately.</li> </ul>	off	—
gummel_acc=<float>	Sets the tolerance to which the current must converge in the Gummel iterations.	1e-4	—
import_bands= off   on	Specifies whether to import band profiles that are in the TDR file (see <a href="#">Importing Conduction Band and Valence Band Information on page 67</a> ). Options are: <ul style="list-style-type: none"> <li>off: Do no import band profiles.</li> <li>on: Import band profiles.</li> </ul>	off	—
import_bands_override=<string>	Specifies the materials and regions in which the imported band parameters should be overridden by the default value or values explicitly set in the input file (see <a href="#">Overriding the Imported Band Parameters on page 68</a> ).	—	—

## Appendix B: Input File Commands

### simulation Command

Parameter	Description	Default	Unit
import_bulk_mobility= off   on	Specifies whether to import mobility as only bulk mobility from the TDR file (see <a href="#">Importing Mobility on page 71</a> ). Options are: <ul style="list-style-type: none"> <li>• off: Do not import mobility as only bulk mobility.</li> <li>• on: Import mobility as only bulk mobility.</li> </ul>	off	—
import_dg_limit= <float>	Sets an upper limit on the value of the density-gradient effective mass that is derived from an imported density-gradient calibration parameter (see <a href="#">Limiting the Imported Density-Gradient Effective Mass on page 70</a> ).	1.0	—
import_dg_override_auto= off   on	Specifies whether to override the imported density-gradient calibration parameter in the channel direction (see <a href="#">Overriding the Imported Density-Gradient Calibration Parameter on page 69</a> ). Options are: <ul style="list-style-type: none"> <li>• off: Do not override the calibration parameter.</li> <li>• on: Override the calibration parameter.</li> </ul>	off	—
import_dg_override_x= off   on	Specifies whether to override the imported density-gradient calibration parameter in the x-direction (see <a href="#">Overriding the Imported Density-Gradient Calibration Parameter</a> ). Options are: <ul style="list-style-type: none"> <li>• off: Do not override the calibration parameter.</li> <li>• on: Override the calibration parameter.</li> </ul>	off	—
import_dg_override_y= off   on	Specifies whether to override the imported density-gradient calibration parameter in the y-direction (see <a href="#">Overriding the Imported Density-Gradient Calibration Parameter</a> ). Options are: <ul style="list-style-type: none"> <li>• off: Do not override the calibration parameter.</li> <li>• on: Override the calibration parameter.</li> </ul>	off	—

## Appendix B: Input File Commands

### simulation Command

Parameter	Description	Default	Unit
import_dg_override _z= off   on	Specifies whether to override the imported density-gradient calibration parameter in the z-direction (see <a href="#">Overriding the Imported Density-Gradient Calibration Parameter</a> ). Options are: <ul style="list-style-type: none"> <li>off: Do not override the calibration parameter.</li> <li>on: Override the calibration parameter.</li> </ul>	off	—
import_dg= off   on	Specifies whether to import the density-gradient calibration parameter (see <a href="#">Importing the Density-Gradient Calibration Parameter on page 68</a> ). Options are: <ul style="list-style-type: none"> <li>off: Do not import the calibration parameter.</li> <li>on: Import the calibration parameter.</li> </ul>	off	—
import_dielectric_ override=<string>	Specifies the materials and regions in which the imported dielectric constant should be overridden by the default value or a value explicitly set in the input file (see <a href="#">Overriding the Imported Dielectric Constant on page 71</a> ).	—	—
import_dielectric= off   on	Specifies whether to import the dielectric constant from the TDR file (see <a href="#">Importing the Dielectric Constant on page 70</a> ). Options are: <ul style="list-style-type: none"> <li>off: Do not import the dielectric constant.</li> <li>on: Import the dielectric constant.</li> </ul>	off	—
import_mobility= off   on	Specifies whether to import mobility fields from the TDR file (see <a href="#">Importing Mobility on page 71</a> ). Options are: <ul style="list-style-type: none"> <li>off: Do not import mobility fields.</li> <li>on: Import mobility fields.</li> </ul>	off	—
import_override= <string>	This parameter is the equivalent of specifying both <code>import_bands_override</code> and <code>import_dielectric_override</code> with the same list of materials or regions.	—	—

## Appendix B: Input File Commands

### simulation Command

Parameter	Description	Default	Unit
import_solution=off   on	<p>Specifies whether to import the solution state from a TDR file. The input TDR file in this case must be the output TDR file produced by a previous Garand simulation (see <a href="#">Importing the Solution From Garand TDR Files on page 73</a>).</p> <p>Options are:</p> <ul style="list-style-type: none"> <li>• off: Do not import the solution.</li> <li>• on: Import the solution.</li> </ul>	off	—
irand0=<integer>	Adds an offset to the initial seed for the random number generators. This results in a different variability configuration for the same device number. The recommended range of values is 0 to 999.	0	—
iter_max=<integer>	Sets the maximum number of Gummel iterations to perform.	100	—
iter_min=<integer>	Sets the minimum number of Gummel iterations to perform. It cannot be less than 3.	3	—
	<b>Note:</b> It is sometimes useful to set this to 20 when running $I_d$ - $V_d$ simulations to avoid false convergence.		
mobility_sweep_mode= grid   points	<p>Specifies the mode in which to run a mobility sweep with multiple mobility parameters.</p> <p>Options are:</p> <ul style="list-style-type: none"> <li>• grid: Run mobility sweep in grid mode.</li> <li>• points: Run mobility sweep in points mode.</li> </ul> <p>See <a href="#">Handling Multiple Mobility Sweeps on page 121</a>.</p>	grid	—
mobility_sweep_target=<float>	Sets the target current you want to find when running a mobility sweep (see <a href="#">Specifying a Target Current on page 121</a> ).	—	A
n_or_p=<string>	<p>Sets the channel type to be simulated. Options are:</p> <ul style="list-style-type: none"> <li>• n: Simulate an n-channel MOSFET.</li> <li>• p: Simulate a p-channel MOSFET.</li> </ul> <p><b>Note:</b> You must specify this parameter in every input file.</p>	—	—

## Appendix B: Input File Commands

### simulation Command

Parameter	Description	Default	Unit
nlimitc_init=<integer>	Sets the maximum number of iterations for the current continuity solver on the first Gummel iteration.	nlimitc	—
nlimitc=<integer>	Sets the maximum number of iterations for the current continuity equation solver.	1000	—
nlimitdg=<integer>	Sets the maximum number of iterations for the density gradient solver.	1000	—
nlimitp_init=<integer>	Sets the maximum number of iterations for the Poisson solver on the first Gummel iteration.	nlimitp	—
nlimitp=<integer>	Sets the maximum number of iterations for the Poisson solver.	1000	—
poisson_nonlinear_update=<integer>	Sets the number of iterations of the successive over-relaxation solver between nonlinear updates.	50	—
poisson_qc_acc=<float>	Sets the tolerance to which the change in either the potential or log carrier concentration, from one iteration to the next iteration, must converge when running with solve=dg or solve=schrod.	5e-3	—
pot_converged= off   on	Specifies whether to enforce that the Poisson equation must reach full convergence before the global solution can be considered converged. Options are: <ul style="list-style-type: none"> <li>• off: Do not enforce that Poisson equation must reach full convergence.</li> <li>• on: Enforce that Poisson equation must reach full convergence.</li> </ul>	off	—
sim_type=<string>	Sets the type of simulation. Options are: <ul style="list-style-type: none"> <li>• idvd: <math>I_d - V_d</math> characteristics</li> <li>• idvg: <math>I_d - V_g</math> characteristics</li> <li>• target: Search for <math>V_g</math> that produces a target current</li> </ul>	idvg	—

## Appendix B: Input File Commands

### simulation Command

Parameter	Description	Default	Unit
solve=<string>	Sets whether to obtain a full drift-diffusion solution, or to solve only the nonlinear Poisson equation, or to have no solution. Options are: <ul style="list-style-type: none"> <li>• dg: Solve the nonlinear Poisson equation and the density gradient equation self-consistently.*</li> <li>• off: Do not solve the drift-diffusion equations.</li> <li>• on: Obtain the full drift-diffusion solution based on the specifications in the input file.</li> <li>• poisson: Perform one single solution of the nonlinear Poisson equation.*</li> <li>• schrod: Solve the nonlinear Poisson equation and the Schrödinger equation self-consistently.*</li> </ul> <p>*Use these options only with zero applied drain bias for reliable results.</p>	on	—
target_acc=<float>	Sets the accuracy to which $V_g$ at the target current should be found when running with <code>sim_type=target</code> .	$10^{-4}$	V
target_current=<float>	Sets the target current when running with <code>sim_type=target</code> .	$10^{-8}$	A
target_init_slope=<float>	Sets the initial subthreshold slope to use to project to the next point when running with <code>sim_type=target</code> .	70.0	mV/decade
target_iter_max=<integer>	Sets the maximum number of search iterations to use when running with <code>sim_type=target</code> .	10	—
target_max_slope=<float>	Sets a maximum limit on the slope that is used to predict the next gate voltage during a target current search.	200	mV/decade

**Note:**

If the subthreshold slope of the simulated device is greater than the default (200 mV/decade), then you should increase this limit.

## Appendix B: Input File Commands

### simulation Command

Parameter	Description	Default	Unit
use_schrod_qc= off   on	If the Schrödinger solution is activated (see <a href="#">Schrödinger Quantum Corrections on page 125</a> ), then this parameter specifies whether to solve the Schrödinger solution self-consistently within the Gummel loop and to use it as a quantum correction. Otherwise, a separate Poisson–Schrödinger solution is performed after an initial drift-diffusion solution. Options are: <ul style="list-style-type: none"> <li>off: Do not use Schrödinger-based quantum corrections.</li> <li>on: Use Schrödinger-based quantum corrections.</li> </ul>	on	—

#### Parameters specific to Garand MC only

abstol=<float>	Sets the upper value of the error in the current that must be achieved before a Monte Carlo simulation is considered converged and execution automatically terminates, assuming convergence within the percentage error has not been satisfied ( $\text{abstol} > 0$ ).	$1 \times 10^{-8}$	A
applied_field=<float> <float> <float>	Sets the driving field along the x-, y-, and z-directions. See <a href="#">Automatically Slicing a Device on page 231</a> .	0.0 0.0 0.0	kV/cm
DT=<float>	Sets the length of the field-adjusting time step ( $\Delta t > 0$ ). The default of 0.05 fs ensures the minimum requirements for numeric accuracy of carrier propagation within a self-consistent quantum-corrected potential.	$5 \times 10^{-17}$	s
electrons= off   on	Specifies whether electrons are resolved as particles and simulated. Options are: <ul style="list-style-type: none"> <li>off: Do not resolve electrons and do not simulate.</li> <li>on: Resolve electrons and simulate.</li> </ul>	off	—
ensemble= off   on	Specifies whether to perform a self-consistent ensemble MC simulation. Options are: <ul style="list-style-type: none"> <li>off: Do not perform a self-consistent ensemble simulation.</li> <li>on: Perform a self-consistent ensemble simulation.</li> </ul>	on	—

## Appendix B: Input File Commands

### simulation Command

Parameter	Description	Default	Unit
holes= off   on	Specifies whether holes are resolved as particles and simulated. Options are: <ul style="list-style-type: none"> <li>• off: Do not resolve holes and do not simulate.</li> <li>• on: Resolve holes and simulate.</li> </ul>	off	—
iter_q_assign=<integer>	Specifies whether to apply charge reassignment. Options are: <ul style="list-style-type: none"> <li>• 0: Do no apply charge reassignment.</li> <li>• 1: Perform a single charge reassignment iteration in regions of high charge density.</li> </ul>	1	—
num_elec_sp=<integer>	Sets the number of independent particles used to simulate electrons in single-particle simulations.	10000	—
num_elec=<integer>	Sets the number of particles used to represent the initial continuous electron distribution ( $0 < \text{num\_elec} \leq 450000$ ). The num_elecs parameter takes a positive integer value with an upper limit of 200 000. This together with the initial total electron charge determines the superparticle charge [1].	200000	—
num_flux=<integer>	Sets the initial period of flux.	10000	—
num_hole_sp=<integer>	Sets the number of independent particles used to simulate holes in single-particle simulations.	10000	—
num_hole=<integer>	Sets the number particles used to represent the initial continuous hole distribution ( $0 < \text{num\_hole} \leq 450000$ ). The num_holes parameter takes a positive integer value with an upper limit of 200 000. This together with the initial total hole charge determines the superparticle charge [1].	200000	—

## Appendix B: Input File Commands

### simulation Command

Parameter	Description	Default	Unit
num_inter=<integer>	Sets the number of time steps between successive intermittent results output ( $\text{num\_inter} > 0$ ).  By default, the number of time steps between successive intermittent outputs is 20000. This together with the default field-adjusting time step gives an intermittent period of 1.0 ps. The start of the first intermittent period coincides with the time step $t = 0$ .	20000	—
num_nlin=<integer>	Sets the number of time steps between successive solutions of the nonlinear Poisson equation, solving both potential and continuous carrier concentration given the fixed carrier concentration from MC particle propagation ( $\text{num\_nlin} > 0$ ).  The default number of time steps between successive nonlinear Poisson solutions is 20000. This together with the default field-adjusting time step gives a period of 1 ps between solutions.	20000	—
num_stats=<integer>	Sets the number of time steps between which successive simulation statistics are gathered ( $\text{num\_stats} > 0$ ).  The default is to gather statistics every 20 time steps, equivalent to every femtosecond given the default field-adjusting time step.	20	—
num_steps=<integer>	Sets the total number of time steps over which to propagate particles in the simulation ( $\text{num\_steps} > 0$ ).  The default of 200000 time steps, with the default field-adjusting time step, gives a default simulation time of 10 ps.	200000	—

## Appendix B: Input File Commands

### simulation Command

Parameter	Description	Default	Unit
num_trans= <integer>	Sets the number of time steps that cover the transient period from the start of the simulation ( <code>num_trans &gt; 0</code> ).  By default, the initial transient period is defined as 40 000 time steps. This together with the default field-adjusting time step gives a default transient period of 2 ps.  This transient period is usually optimal for default silicon at 300 K, but it might need to be extended for materials, or under conditions, in which the relaxation time is longer.	40000	—
ohm_ctc= off   on	Specifies whether to include particle injection and removal at Ohmic contacts Options are: <ul style="list-style-type: none"><li>• off: Do not include particle injection and removal.</li><li>• on: Include particle injection and removal.</li></ul>	on	—
periodicX= off   on	Specifies whether to set the external boundaries to be periodic in the x-direction. <ul style="list-style-type: none"><li>• off: Do not set periodic external boundaries.</li><li>• on: Set periodic external boundaries.</li></ul>	off	—
periodicY= off   on	Specifies whether to set the external boundaries to be periodic in the y-direction. <ul style="list-style-type: none"><li>• off: Do not set periodic external boundaries.</li><li>• on: Set periodic external boundaries.</li></ul>	off	—
periodicZ= off   on	Specifies whether to set the external boundaries to be periodic in the z-direction. <ul style="list-style-type: none"><li>• off: Do not set periodic external boundaries.</li><li>• on: Set periodic external boundaries.</li></ul>	off	—
reflect_ext = off   on	Specifies the boundary conditions to use at external boundaries (see <a href="#">External Boundaries on page 261</a> ). Options are: <ul style="list-style-type: none"><li>• off: Use internal boundary conditions at external boundaries.</li><li>• on: Use external boundary conditions at external boundaries.</li></ul>	on	—

## Appendix B: Input File Commands

### simulation Command

Parameter	Description	Default	Unit
self_consistent= off   on	Specifies whether to perform carrier propagation within a self-consistent potential. Options are: <ul style="list-style-type: none"><li>• off: Do not perform carrier propagation within a self-consistent potential. The MC simulation uses the frozen-field approximation.</li><li>• on: Perform carrier propagation within a self-consistent potential.</li></ul>	on	—
single_particle= off   on	Specifies whether to perform a single-particle, frozen-field, MC simulation. Options are: <ul style="list-style-type: none"><li>• off: Do not perform a single-particle simulation.</li><li>• on: Perform a single-particle simulation.</li></ul>	off	—
superparticles= off   on	Specifies whether particles resolving the initial continuous carrier distribution can have a nonunity electronic charge. Options are: <ul style="list-style-type: none"><li>• off: Particles cannot have a nonunity electronic charge.</li><li>• on: Particles can have a nonunity electronic charge.</li></ul>	on	—
tolerance=<float>	Sets the upper value of the percentage error in the current that must be achieved before a MC simulation is considered converged and execution terminates automatically ( $0 < \text{tolerance} \leq 100$ ).	5.0	%

---

## Internal Sweep of Mobility Parameters

You can specify a material mobility parameter and a list of values over which it will be swept. See [Internal Sweep of Mobility Parameters on page 120](#).

### Syntax

```
simulation mobility_sweep parameter=<string> values=<list>
```

## Appendix B: Input File Commands

### strain command

Parameter	Description	Default	Unit
parameter=<string>	Sets the full hierarchical material mobility parameter whose value should be swept.	–	–
values=<list>	Specifies a comma-separated list of mobility parameter values.	–	–

### strain command

This command specifies settings with regard to importing strain fields from process simulations.

The `strain` command can also be used to define sources of stress or strain by using the input file (see [Material Strain on page 285](#)).

#### Syntax

```
strain <parameter>=<value>
```

Parameter	Description	Default	Unit
<b>Parameters common to Garand and Garand MC</b>			
import= off   on	Specifies whether to include strain effects from an imported stress tensor (see <a href="#">Importing a Stress Tensor on page 94</a> ). Options are: <ul style="list-style-type: none"><li>• off: Do not include strain effects.</li><li>• on: Include strain effects.</li></ul>	off	–
<b>Parameters specific to Garand MC only</b>			
additive= off   on	Specifies whether to add definitions of stress in the input file to averaged values transferred from a drift-diffusion simulation (see <a href="#">Applying Stress on page 229</a> ). Options are: <ul style="list-style-type: none"><li>• off: Do not sum stress.</li><li>• on: Sum stress sources.</li></ul>	off	–

## Appendix B: Input File Commands

### structure Command

Parameter	Description	Default	Unit
diagonal_only= off   on	Specifies whether to transfer only the diagonal components of the stress tensor for each region from drift-diffusion to Monte Carlo simulations (see <a href="#">Applying Stress on page 229</a> ). Options are: <ul style="list-style-type: none"><li>• off: Transfer all stress tensor components.</li><li>• on: Transfer only the diagonal components (XX, YY, and ZZ).</li></ul>	off	—
transfer_average= off   on	Specifies whether to transfer the average stress in each region from drift-diffusion to Monte Carlo simulation (see <a href="#">Applying Stress on page 229</a> ). Options are: <ul style="list-style-type: none"><li>• off: Do not transfer the average stress.</li><li>• on: Transfer the average stress.</li></ul>	off	—

## structure Command

This command specifies various device structure options for Garand.

### Note:

All commands in this section apply only to Garand.

### Syntax

```
structure <parameter>=<value>
```

Import a device structure (see [Importing Structures From TDR Files on page 51](#)):

```
structure import filename=<string>
```

Reflect an imported device structure (see [Reflecting Imported Device Structures on page 60](#)):

```
structure reflect x+ | x- | y+ | y- | z+ | z- = on | off
```

Change materials (see [Changing Materials on page 76](#)):

```
structure replace tdr_mat=<string> garand_mat=<string>
```

```
structure replace region=<string> garand_mat=<string>
```

```
structure replace mat1=<string> mat2=<string>
```

## Appendix B: Input File Commands

### structure Command

Add a uniform fixed charge (see [Adding a Uniform Fixed Charge on page 904](#))

```
structure add_charge density=<float> \
    [material=<string>] [region=<string>] \
    [xmin=<float>] [xmax=<float>] \
    [ymin=<float>] [ymax=<float>] \
    [zmin=<float>] [zmax=<float>]
```

Add a user-defined region to a device structure (see [Adding User-Defined Regions on page 62](#)):

```
structure add_region name=<string> material=<string> \
    [new_material=<string>] \
    [xmin=<float>] [xmax=<float>] \
    [ymin=<float>] [ymax=<float>] \
    [zmin=<float>] [zmax=<float>]
```

Parameter	Description	Default	Unit
acceptor_fields=<string>	Sets a comma-separated list of acceptor doping fields to import from the TDR file.	—	—
areafactor=<float>	Sets a scaling factor that multiplies the current output.	1.0	—
channel_dir=<string>	Sets the channel direction. Options are: <ul style="list-style-type: none"><li>• x</li><li>• y</li><li>• z</li></ul>	—	—
donor_fields=<string>	Sets a comma-separated list of donor doping fields to import from the TDR file.	—	—
erode_sd=<float>	Specifies to replace semiconductor material in source/drain with metallic contact if doping is greater than or equal to this value and the point is physically connected by at least this level of doping to the existing source/drain contact.	—	cm <sup>-3</sup>
extra_doping_from_net= off   on	Specifies whether to compare the doping obtained from dopant species fields with the net doping from the DopingConcentration field. Options are: <ul style="list-style-type: none"><li>• off: Exclude any extra doping found in DopingConcentration.</li><li>• on: Include any extra doping found in DopingConcentration.</li></ul>	on*	—

\*This is set automatically to off if you specify acceptor\_fields or donor\_fields.

## Appendix B: Input File Commands

### structure Command

Parameter	Description	Default	Unit
filename=<string>	Sets the name of the TDR file from which to import a structure. This parameter applies to <code>structure import</code> commands (see <a href="#">Importing Structures From TDR Files on page 51</a> ).	—	—
garand_mat=<string>	Sets the name of a valid material in Garand. This parameter applies to <code>structure replace</code> commands (see <a href="#">Changing Materials on page 76</a> ).	—	—
gate_length=<float>	Sets a fixed gate length to be used in reference calculations.	—	Input unit <sup>1</sup>
input_units=<string>	Sets the unit for simulation input only. Options are: <ul style="list-style-type: none"><li>• nm</li><li>• um</li><li>• mm</li><li>• cm</li><li>• m</li></ul> This parameter overrides any unit set with the <code>units</code> parameter.	nm	—
limit_sd_doping=<float>	Sets the doping concentration to use if <code>limit_sd=doping</code> .	$10^{17}$	$\text{cm}^{-3}$
limit_sd=<string>	Sets the method used to determine the source and drain regions if the channel doping is so low that there is no p-n junction between the source and drain. Options are: <ul style="list-style-type: none"><li>• <code>doping</code>: Use a doping concentration to define the limit of the source and drain regions.</li><li>• <code>middle</code>: Use the middle of the simulation structure in the channel direction.</li></ul>	middle	—
mat1=<string>	Sets the name of a material to be changed. This parameter applies to <code>structure replace</code> commands (see <a href="#">Changing Materials Globally on page 77</a> ).	—	—

## Appendix B: Input File Commands

### structure Command

Parameter	Description	Default	Unit
mat2=<string>	Sets the name of the material that will replace the material set in mat1. This parameter applies to structure replace commands (see <a href="#">Changing Materials Globally on page 77</a> ).	–	–
material=<string>	Sets the current material within elements to be added to the new region.	–	–
max_stress=<float>	Sets the maximum limit imposed on the stress in the structure.	$4 \times 10^9$	Pa
mct_file=<string>	Sets the name of the Monte Carlo transfer file.	–	–
min_eg=<float>	Sets the minimum limit on the band gap in the device structure.	0.1	eV
name=<string>	Sets the name of the new region.	–	–
new_material=<string>	Sets a different material for the new region.	–	–
region=<string>	Sets the name of a region in the TDR file. This parameter applies to structure replace commands (see <a href="#">Changing Materials in Regions on page 77</a> ).	–	–
remove_source_drain = off   on	Specifies whether to remove the heavily doped source/drain regions to allow for long-channel simulations. This parameter applies only to FinFET and nanowire architectures. Options are: <ul style="list-style-type: none"><li>• off: Do not remove heavily doped source/drain regions.</li><li>• on: Remove heavily doped source/drain regions.</li></ul>	off	–
restrict_eroe_sd=off   on	Specifies whether to restrict the erosion of the source/drain such that the redefinition to a metallic contact is restricted to the user-defined bounding box defining a contact. Options are: <ul style="list-style-type: none"><li>• off: Do not restrict erosion of source/drain.</li><li>• on: Restrict erosion of source/drain.</li></ul>	off	–

## Appendix B: Input File Commands

### structure Command

Parameter	Description	Default	Unit
tdr_mat=<string>	Sets the name of a material used in the TDR file.  This parameter applies to <code>structure replace</code> commands (see <a href="#">Changing Materials on page 76</a> ).	—	—
units=<string>	Sets the unit for both simulation input and output. Options are: <ul style="list-style-type: none"><li>• nm</li><li>• um</li><li>• mm</li><li>• cm</li><li>• m</li></ul>	—	—
x+   x-   y+   y-   z+   z- = [on   off]	Sets the direction in which to reflect an imported device structure. These parameters apply to <code>structure reflect</code> commands (see <a href="#">Reflecting Imported Device Structures on page 60</a> ).	—	—
xmax=<float>	Sets the maximum extent of the bounding box in the x-direction.	—	Input unit <sup>1</sup>
xmin=<float>	Sets the minimum extent of the bounding box in the x-direction.	—	Input unit <sup>1</sup>
xMoleFraction= off   on	Specifies whether to import the <code>xMoleFraction</code> field from the TDR file (see <a href="#">Importing an Alloy Fraction on page 90</a> ). Options are: <ul style="list-style-type: none"><li>• off: Do not import the <code>xMoleFraction</code> field.</li><li>• on: Import the <code>xMoleFraction</code> field.</li></ul>	on	—
ymax=<float>	Sets the maximum extent of the bounding box in the y-direction.	—	Input unit <sup>1</sup>
ymin=<float>	Sets the minimum extent of the bounding box in the y-direction.	—	Input unit <sup>1</sup>

## Appendix B: Input File Commands

### structure Command

Parameter	Description	Default	Unit
<code>zmax=&lt;float&gt;</code>	Sets the maximum extent of the bounding box in the z-direction.	–	Input unit <sup>1</sup>
<code>zmin=&lt;float&gt;</code>	Sets the minimum extent of the bounding box in the z-direction.	–	Input unit <sup>1</sup>

1. The default input unit for Garand is the nanometer, but it can be changed (see [Dimensional Unit on page 45](#)).

---

## Importing Alloy Fractions

You can change the default mapping of alloy fractions for SiGe where spatial variation of parameters is deactivated (see [Importing an Alloy Fraction on page 90](#)).

### Syntax

```
structure define_sige <parameter>=<value> <parameter1>=<value1> ...
```

Parameter	Description	Default	Unit
<code>ge_x_max=&lt;float&gt;</code>	Sets the upper value for the alloy fraction (between 0 and 1).	0.0	–
<code>ge_x_min=&lt;float&gt;</code>	Sets the lower value for the alloy fraction (between 0 and 1).	0.0	–
<code>mat=&lt;string&gt;</code>	Sets the name of the material to be used within a given range.	–	–

---

## Adding a Uniform Fixed Charge

You can add a region of uniform fixed charge to the simulation structure (see [Adding a Uniform Fixed Charge on page 90](#)).

### Syntax

```
structure add_charge density=<float> \
    [material=<string>] [region=<string>] \
    [xmin=<float>] [xmax=<float>] \
    [ymin=<float>] [ymax=<float>] \
    [zmin=<float>] [zmax=<float>]
```

## Appendix B: Input File Commands

### structure Command

Parameter	Description	Default	Unit
density=<float>	Sets the volume density of charge to be added. This density is signed, which means: <ul style="list-style-type: none"><li>• A positive density adds a positive charge.</li><li>• A negative density adds a negative charge.</li></ul>	0 . 0	cm <sup>-3</sup>
material=<string>	Specifies a comma-separated list of materials that restricts the materials in which charge is added.	—	—
region=<string>	Specifies a comma-separated list of regions that restricts the regions in which charge is added.	—	—
xmax=<float>	Sets the maximum extent of the bounding box for the added charge in the x-direction.	—	Input unit <sup>1</sup>
xmin=<float>	Sets the minimum extent of the bounding box for the added charge in the x-direction.	—	Input unit <sup>1</sup>
ymax=<float>	Sets the maximum extent of the bounding box for the added charge in the y-direction.	—	Input unit <sup>1</sup>
ymin=<float>	Sets the minimum extent of the bounding box for the added charge in the y-direction.	—	Input unit <sup>1</sup>
zmax=<float>	Sets the maximum extent of the bounding box for the added charge in the z-direction.	—	Input unit <sup>1</sup>
zmin=<float>	Sets the minimum extent of the bounding box for the added charge in the z-direction.	—	Input unit <sup>1</sup>

1. The default input unit for Garand is the nanometer, but it can be changed (see [Dimensional Unit on page 45](#)).

## Appendix B: Input File Commands

### variability Command

---

## variability Command

This command specifies the options for various statistical variability sources (see [Statistical Variability Sources on page 100](#)).

#### Note:

All commands in this section apply only to Garand.

#### Syntax

```
variability <variability_source> <parameter>=<value>
```

The available variability sources are:

- [Random Discrete Dopants](#)
- [Line Edge Roughness](#)
- [Metal Gate Granularity](#)
- [Polysilicon Gate Granularity](#)

---

## Random Discrete Dopants

You can specify that random discrete dopants (RDD) should be generated automatically, based on the nominal continuous doping profiles (see [Random Discrete Dopants on page 100](#)). In addition, you can import the exact locations of random discrete dopants by using the `import` option (see [Importing Positions of Random Discrete Dopants on page 102](#)).

#### Syntax

```
variability RDD <parameter>=<value>
```

Parameter	Description	Default	Unit
<code>status= off   on</code>	Specifies whether to include random discrete dopants in the simulation. Options are: <ul style="list-style-type: none"><li>• <code>off</code>: Do not include random discrete dopants, that is, use continuous doping.</li><li>• <code>on</code>: Include random discrete dopants.</li></ul>	<code>off</code>	—
<code>acceptor_fields= &lt;string&gt;</code>	Sets a comma-separated list of imported acceptor dopant fields to be converted to discrete dopants.	—	—
<code>donor_fields= &lt;string&gt;</code>	Sets a comma-separated list of imported donor dopant fields to be converted to discrete dopants.	—	—

## Appendix B: Input File Commands

### variability Command

Parameter	Description	Default	Unit
dopants=<string>	Sets which doping will be discrete. Options are: <ul style="list-style-type: none"> <li>• all: All doping is discrete.</li> <li>• acceptors: Only acceptor doping is discrete.</li> <li>• donors: Only donor doping is discrete.</li> </ul>	all	—
include_poly= off   on	Specifies whether to generate discrete dopants in polysilicon gates (see <a href="#">RDD in Polysilicon Gates on page 102</a> ). Options are: <ul style="list-style-type: none"> <li>• off: Do not generate discrete dopants.</li> <li>• on: Generate discrete dopants.</li> </ul>	on	—
mob_comp= off   on	Specifies whether to activate mobility compensation for discrete doping in source/drain regions. Options are: <ul style="list-style-type: none"> <li>• off: Do not activate mobility compensation.</li> <li>• on: Activate mobility compensation.</li> </ul>	on	—
separate_species = off   on	Specifies whether to consider RDD generation for each species field separately. Options are: <ul style="list-style-type: none"> <li>• off: RDD considers acceptors and donors (original method).</li> <li>• on: RDD considers species fields separately.</li> </ul>	off	—
write_positions= off   on	Specifies whether to write the positions of random discrete dopants to a text file. Options are: <ul style="list-style-type: none"> <li>• off: Do not write RDD positions to file.</li> <li>• on: Write RDD positions to file.</li> </ul>	off	—
xmin=<float>	Sets the lower x-boundary of the RDD region for imported structures.	Minimum x-boundary	Input unit <sup>1</sup>
xmax=<float>	Sets the upper x-boundary of the RDD region for imported structures.	Maximum x-boundary	Input unit <sup>1</sup>
ymin=<float>	Sets the lower y-boundary of the RDD region for imported structures.	Minimum y-boundary	Input unit <sup>1</sup>
ymax=<float>	Sets the upper y-boundary of the RDD region for imported structures.	Maximum y-boundary	Input unit <sup>1</sup>
zmin=<float>	Sets the lower z-boundary of the RDD region for imported structures.	Minimum z-boundary	Input unit <sup>1</sup>

## Appendix B: Input File Commands

### variability Command

Parameter	Description	Default	Unit
zmax=<float>	Sets the upper z-boundary of the RDD region for imported structures.	Maximum z-boundary	Input unit <sup>1</sup>

1. *The default input unit for Garand is the nanometer, but it can be changed (see Dimensional Unit on page 45).*

## Importing Positions of Random Discrete Dopants

You can import dopant positions (see [Importing Positions of Random Discrete Dopants on page 102](#)).

### Syntax

```
variability RDD import <parameter>=<value>
```

Parameter	Description	Default	Unit
field=<string>	Sets the impurity atom field to read in from the KMC defects file.	–	–
file=<string>	Sets the name of a file containing the discrete dopant positions.	–	–
species=<string>	Sets the discrete dopant family. Options are: <ul style="list-style-type: none"><li>• acceptors</li><li>• donors</li></ul>	–	–
units=<string>	Sets the physical unit in which the positions are given. Options are: <ul style="list-style-type: none"><li>• m: Meter</li><li>• cm: Centimeter</li><li>• mm: Millimeter</li><li>• um: Micrometer</li><li>• nm: Nanometer</li></ul> It is advisable to always specify the units.	nm	–

## Appendix B: Input File Commands

### variability Command

---

## Line Edge Roughness

This variability type specifies that line edge roughness (LER) is applied to a particular part of the device structure, and all options for this particular roughness are supplied in the same command line in the input file. This is because LER can be applied in multiple directions simultaneously. See [Line Edge Roughness on page 105](#).

### Syntax

```
variability LER <parameter1>=<value1> <parameter2>=<value2> ...
```

Parameter	Description	Default	Unit
status= off   on	Specifies whether to include this LER specification in the simulation. Options are: <ul style="list-style-type: none"><li>• off: Do not include LER.</li><li>• on: Include LER.</li></ul>	off	—
corr=<float>	Sets the correlation length of the random lines used in LER.	30.0	nm
correlated= off   on	Specifies whether to correlate the applied LER, that is, to use the same random line on both sides of the specified midpoint. Options are: <ul style="list-style-type: none"><li>• off: Do not correlate the applied LER, that is, uncorrelated.</li><li>• on: Correlate the applied LER.</li></ul>	off	—
dir=<string>	Sets the direction in which LER propagates. This will be one of the directions of the plane specified by the midpoint. Options are: <ul style="list-style-type: none"><li>• x</li><li>• y</li><li>• z</li></ul>	—	—
<b>Note:</b>			
You must specify this parameter.			
lww=<float>	Applies an additional Gaussian line width variation, with specified standard deviation.	Not applied	nm
na_rolloff=<float>	Sets the distance from the midpoint from which acceptor doping is projected when constructing overlapping single-sided doping profiles.	Not applied	nm

## Appendix B: Input File Commands

### variability Command

Parameter	Description	Default	Unit
nd_rolloff=<float>	Sets the distance from the midpoint from which donor doping is projected when constructing overlapping single-sided doping profiles.	Not applied	nm
rms=<float>	Sets the root mean square (RMS) amplitude of the random lines used for LER.	0.0	nm
uniform=<float>	Applies LER with a uniform profile that moves the gate edges outwards for positive values and inwards for negative values.	Not applied	nm
<b>Note:</b>	This parameter overrides any specification of <code>rms</code> and <code>corr</code> .		
x   y   z =<float>	Sets the position of the midpoint of the LER in the direction in which the roughness will be applied, that is, perpendicular to the random line.	-	Input unit <sup>1</sup>
<b>Note:</b>	You must specify one of these parameters.		

1. The default input unit for Garand is the nanometer, but it can be changed (see [Dimensional Unit on page 45](#)).

---

## Metal Gate Granularity

You can specify metal gate granularity (MGG). See [Metal Gate Granularity on page 110](#).

### Syntax

```
variability MGG <parameter>=<value>
```

Parameter	Description	Default	Unit
status= off   on	Specifies whether to include MGG in the simulation. Options are: <ul style="list-style-type: none"><li>• off: Do not include MGG.</li><li>• on: Include MGG.</li></ul>	off	-
diameter=<float>	Sets the average diameter of the metal grains to be used.	5.0	nm

## Appendix B: Input File Commands

### variability Command

Parameter	Description	Default	Unit
packing_density=<float>	When calculating the average grain volume as the volume of a sphere with the given average diameter, use this packing density for those spheres when calculating the average number of grains that will fill the bounding box.  <b>Note:</b> This parameter can take a value such that $0.0 < \text{packing\_density} \leq 1.0$ .	1.0	-
volume_rsd=<float>	Sets the relative standard deviation of the sphere volume for the grain generation using a Voronoï pattern in Laguerre geometry.	0.0	-

## Adding Metal Gate Grains

You can add metal gate grains (see [Adding Metal Gate Grains on page 111](#)).

### Syntax

```
variability MGG add_grain <parameter>=<value>
```

Parameter	Description	Default	Unit
add_grain	With this option, you can add a grain orientation to the MGG. It requires the following parameters to be set: <ul style="list-style-type: none"><li>• wf_delta <b>or</b> workfunction</li><li>• probability</li></ul> <b>Note:</b> You cannot specify both workfunction and wf_delta in the same command.	-	-
probability=<float>	Sets the probability (between 0.0 and 1.0) for the grain orientation to occur.	-	-
wf_delta=c	Sets the workfunction for the grain orientation as an offset from the specified nominal workfunction.	-	eV
workfunction=<float>	Sets the workfunction for the grain orientation.	-	eV

## Appendix B: Input File Commands

### variability Command

---

## Polysilicon Gate Granularity

You can specify polysilicon gate granularity (PGG). See [Polysilicon Gate Granularity on page 112](#).

### Syntax

```
variability PGG <parameter>=<value>
```

---

Parameter	Description	Default	Unit
status= off   on	Specifies whether to include Fermi-level pinning due to PGG in the simulation. Options are: <ul style="list-style-type: none"><li>• off: Do not include PGG.</li><li>• on: Include PGG.</li></ul>	off	—
diameter=<float>	Sets the average diameter of the polysilicon grains.	40	nm
packing_density=<float>	When calculating the average grain volume as the volume of a sphere with the given average diameter, use this packing density for those spheres when calculating the average number of grains that will fill the bounding box. <b>Note:</b> This parameter can take a value such that $0.0 < \text{packing\_density} \leq 1.0$ .	1.0	—
pinning=<float>	Sets the trap level within the energy gap at which the Fermi level must be pinned along the polysilicon grain boundaries. This is specified as eV below the conduction band edge.	0.3	eV
volume_rsd=<float>	Sets the relative standard deviation of the sphere volume for the grain generation using a Voronoï pattern in Laguerre geometry.	0.0	—

---

## Appendix B: Input File Commands

### variability Command

---

## Random Telegraph Noise

You can specify random telegraph noise (RTN). See [Random Telegraph Noise on page 115](#).

### Syntax

```
variability RTN <parameter>=<value>
```

Parameter	Description	Default	Unit
status= off   on	Specifies whether to switch on RTN in the simulation. Options are: <ul style="list-style-type: none"><li>• off: Do not include RTN.</li><li>• on: Include RTN.</li></ul>	off	-
expected_number= <integer>	With the default value, exactly one trap is added. If any other positive integer is specified, then the number of traps to add is taken randomly from a Poisson distribution with that expected number.	1	-
material= <string>	By default, RTN traps can be generated in all semiconductor-insulator interfaces within the bounding box. This parameter allows the semiconductor to be restricted to a specified list of materials. The parameter value should be a comma-separated list of material names.	-	-
num_configs= <integer>	By specifying a positive integer value for this parameter, you can control how many different consecutive random trap positions are considered within a single simulation run.	1	-
oxide_region= <string>	By default, RTN traps can be generated in all semiconductor-insulator interfaces within the bounding box. This parameter allows the insulator to be restricted to a specified list of oxide regions. The parameter value should be a comma-separated list of region names.	-	-
region=<string>	By default, RTN traps can be generated in all semiconductor-insulator interfaces within the bounding box. This parameter allows the semiconductor to be restricted to a specified list of semiconductor regions. The parameter value should be a comma-separated list of region names.	-	-

## Appendix B: Input File Commands

### References

Parameter	Description	Default	Unit
seed=<integer>	By specifying a positive integer value for this parameter, a different position for a single RTN trap can be generated for the same statistical device number.	1	—
xmax=<float>	Sets the maximum extent of the bounding box for the RTN trap in the x-direction.	—	Input unit <sup>1</sup>
xmin=<float>	Sets the minimum extent of the bounding box for the RTN trap in the x-direction.	—	Input unit <sup>1</sup>
ymax=<float>	Sets the maximum extent of the bounding box for the RTN trap in the y-direction.	—	Input unit <sup>1</sup>
ymin=<float>	Sets the minimum extent of the bounding box for the RTN trap in the y-direction.	—	Input unit <sup>1</sup>
zmax=<float>	Sets the maximum extent of the bounding box for the RTN trap in the z-direction.	—	Input unit <sup>1</sup>
zmin=<float>	Sets the minimum extent of the bounding box for the RTN trap in the z-direction.	—	Input unit <sup>1</sup>

1. The default input unit for Garand is the nanometer, but it can be changed (see [Dimensional Unit on page 45](#)).

---

## References

- [1] R. W. Hockney and J. W. Eastwood, *Computer Simulation Using Particles*, New York: Taylor & Francis, 1988.

# C

## Deprecated Input Commands

---

*This appendix presents deprecated input commands.*

---

### Crystal Orientation

Using either `chan` or `sub` as indirect references to the x-axis and z-axis of the simulation domain, used to define reference directions to align crystal lattice orientations, is deprecated.

Instead, use the `x`, `y`, and `z` references explicitly. For example:

```
material Silicon.crystal.x 1 1 0
material Silicon.crystal.y -1 1 0
material Silicon.crystal.z 0 0 1
```

Only two orthogonal directions need to be specified, because the third direction is uniquely defined as being orthogonal to the other two.

To update existing input files, replace `chan` with `x` and `sub` with `z`. For example, the following commands:

```
material Silicon.crystal.chan 1 1 0
material Silicon.crystal.sub 0 0 1
```

would change to:

```
material Silicon.crystal.x 1 1 0
material Silicon.crystal.z 0 0 1
```

---

### Time Series Files

Following the deprecation of VTK file output, the output of time series files for visualization is deprecated.

## Appendix C: Deprecated Input Commands

### Integration of Stress Field

---

## Integration of Stress Field

In previous versions, the stress tensor was averaged in semiconductor materials through the source, channel, and drain by default, and it was modified by using the following parameters:

```
output stress_integration_xmin=<float> stress_integration_xmax=<float>
output stress_integration_ymin=<float> stress_integration_ymax=<float>
output stress_integration_zmin=<float> stress_integration_zmax=<float>
```

These parameters can no longer be defined because the stress is now averaged within each region individually. Therefore, the region where stress is averaged can be controlled using definitions in the input file and modifying the bounds of the regions themselves.

---

## Position-Dependent Parameter for Monte Carlo Simulations

The specific parameter for controlling spatially varying parameters in Monte Carlo simulations is deprecated:

```
simulation mc_pos_dep = on
```

You can control spatially varying parameters by using a common parameter for both Garand and Garand MC:

```
simulation pos_dep = on
```

---

## Setting SiGe-Specific Material Parameters

Using the `fixed_fraction` option is deprecated. It is included only for backward compatibility purposes.

By default, parameters for alloy materials are calculated based on the imported spatially varying mole fraction field. If this is deactivated, then fixed fraction materials are created as described in [Chapter 2 on page 51](#). For SiGe, parameters are controlled using the `SiliconGermanium` material name, but you can control parameters directly using fixed fraction material names.

For example, the following command allows parameters for the `Si70Ge30` material to be defined using that material name:

```
material Si70Ge30.parameters fixed_fraction
```

Then, parameters can be modified in the following way:

```
material SiliconGermanium.permittivity 4.0
material Si70Ge30.permittivity 5.0
```

## **Appendix C: Deprecated Input Commands**

### Setting SiGe-Specific Material Parameters

```
material Silicon_1.permittivity 6.0
material Silicon_1_Si70Ge30.permittivity 7.0
```

In this case, all  $\text{Si}_{1-x}\text{Ge}_x$  materials will have a permittivity of 4.0, with the exception of Si70Ge30, and the Silicon\_1 region again will be further altered, following the same precedence as before.

# Glossary

---

**Bi-CGSTAB**

Bi-conjugate gradient stabilized (Bi-CGSTAB) solver.

**CIC**

Cloud-in-cell.

**DG**

Density gradient.

**DOS**

Density-of-states.

**EMA**

Effective mass approximation.

**EOT**

Equivalent oxide thickness.

**FD**

Finite difference.

**FE**

Finite element.

**ITC**

Interface-trapped charges.

**KMC**

Kinetic Monte Carlo.

**LER**

Line edge roughness.

**MCT file**

Monte Carlo transfer file.

**MGG**

Metal gate granularity.

**NBC**

Neumann boundary conditions.

**NBTI**

Negative bias temperature instability.

**NEC**

Nearest-element-center.

## Glossary

**NEGF**

Non-equilibrium Green's function.

**SOR**

Successive over-relaxation (solver).

**PBTI**

Positive bias temperature instability.

**PDE**

Partial differential equation.

**PDK**

Process design kit.

**QM**

Quantum-mechanical.

**RDD**

Random discrete dopant.

**RMS**

Root mean square.

**RTN**

Random telegraph noise.

**SRH**

Shockley–Read–Hall (generation–recombination).

**TAT**

Trap-assisted tunneling.

**TDR**

File format used for TCAD Sentaurus tools.

**WKB**

Wentzel–Kramers–Brillouin (approximation).

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---

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