MicroTec

Software Package for Two-Dimensional Process and Device Simulation

Version 3.02 for Windows

User's Manual

Siborg Systems Inc

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SRH: Shockley-Read-Hall recombination parameters 80

AUGE: Auger recombination parameters 82 SURF: Surface recombination parameters 82 RADI: Radiative recombination parameters 82

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GETTING STARTED

Chapter 1 Getting Started

1.1. Introduction

Semiconductor device modeling has become a standard design tool in the microelectronics industry. A few years ago this modeling was performed primarily on supercomputers. At the present time a number of commercial 2D process and device simulators are available, mostly for UNIX based workstations. Normally they require tens of Mbytes of memory even for modest size meshes.

Increasing performance and wide spread availability of IBM PCs and compatibles encourage the development of software tools that can be used for 2D modeling of semiconductor devices and processes with a rather low memory capacity and speed of computation. Recently a few efficient programs were developed for two-dimensional semiconductor process-device simulation on a PC which have now been integrated together into a package named **MicroTec**.

MicroTec: The Semiconductor TCAD Calculator

MicroTec allows 2D silicon process modeling including implantation, diffusion and oxidation and 2D steady-state semiconductor device simulation like MOSFET, DMOS, JFET, BJT, IGBT, Schottky, photosensitive devices etc. Although **MicroTec** is significantly simplified compared to widely available commercial simulators, it nevertheless is a very powerful modeling tool for industrial semiconductor process/device design. In many instances **MicroTec** outperforms existing commercial tools and it is remarkably robust and easy-to-use.

MicroTec is especially attractive for educational purposes due to its ease of use and robustness. It enables development of a set of problems for a tutorial in semiconductor device physics with minimal effort. The goal of such a computer-aided course would be to give students basic ideas about modern semiconductor device design. A flexible and easy-to use graphic interface allows the user to output results of the process/device simulation on essentially any printer or plotter or into a file.

Despite apparent simplicity **MicroTec** covers all basic needs for semiconductor process/device design complemented with efficient and flexible graphics tools. It is much easier to use than any other tool of its kind. **MicroTec** is a must for those who want to understand physics of semiconductor devices without knowing much about computers or numerical methods and who do not have much time for learning new process/device simulation tools. **MicroTec** is an excellent tool for managers, R&D engineers, students, professors and researchers and can be referred to as a TCAD calculator.

MicroTec is based on the diffusion-drift model and the present version does not include energy balance. It employs finite-difference technique on a rectangular, auto-adjusting mesh. Only steady-state analysis is available in the present version of **MicroTec**. Physical models (mobility, life time, recombination and impact ionization) implemented in **MicroTec** are essentially the same as those used in the widely used commercial simulators.

Technical Parameters

MicroTec-3.02 is a true 32-bit Windows application and can be run on any PC-386 or higher.

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MicroTec-3.02 uses dynamic memory allocation. There is no memory threshold so it can be used even on a computer with only 1 Mbyte memory if the mesh size is not larger than about 2,000 nodes. Other commercially available tools typically require about 20 Mbyte memory for a mesh size limited by 3,500 nodes. **MicroTec**-3.02 device simulation tools require about 8 Mbytes of memory for a 20,000 node mesh. Typical CPU time for one IV point is less than 1 minute on a PC/486 when using 1,000 nodes. For the process simulation tool, about 4 Mbytes of memory is required for a 20,000 node mesh. Simulation of a typical technological route requires 1-10 minute CPU time on a PC/486.

The most remarkable features of **MicroTec** are: dramatically reduced required memory, absolute numerical stability (almost arbitrary changes of contact voltages, even with impact ionization), high speed and very easy-to-use Graphical User Interface.

1.2. Installing MicroTec

Read about the latest changes in the Installation procedure in the readme.txt file on the installation Disk. You would need about 4 Megabytes of disk space to install **MicroTec**-3.02. If your system is Windows'95, reboot the computer in DOS mode before the installation. If your system is Windows NT, refer to read_nt.txt file on the floppy disk.

- 1. Insert **MicroTec** Disk into a floppy drive.
- 2. Change your current drive to the floppy drive.
- 3. Type "install" and press <Enter>. File "INST.PAS" will be created on the floppy disk.
- 4. Create directory C:\MICROTEC on your hard disk.
- 5. Copy all files from the Disk into this directory.
- 6. Change your current directory to C:\MICROTEC type "pkunzip mt302.zip" and press <Enter>.
- 7. If you have a multiple copy **MicroTec** floppy installation disk repeat steps 1-6 on other computers.

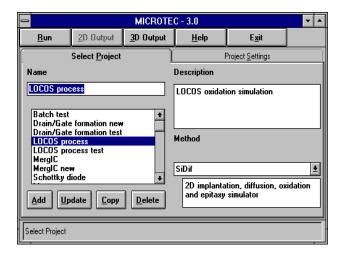
Note: When installing the floppy disk must be open for writing.

1.3. Quick start

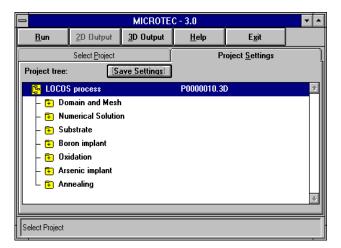
Select a project in the project list window on the "Select Project" page by clicking the left mouse button at the project name. The corresponding simulator name will be shown in the "Method" window. The simulator name may be: SiDif, MergIC, SemSim or Batch for the process simulation, generation of the device structure, device simulation or a batch mode simulation respectively.

In the batch mode you may run a batch of jobs using different tools, for example to run a process simulation, a generation of the final device structure using **MergIC** and then a device simulation for the generated device with a number of different IV curves.

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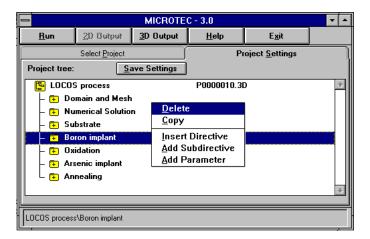


To modify project settings click on "**Project Settings**" tab. Another page of the main **MicroTec** window will appear showing a list of directives, subdirectives and parameters. Click on a folder symbol to open it. Double-click a parameter to edit it.



If you click a directive/subdirective/parameter by the left and then the right mouse button a new window pops up allowing you to "**Delete, Copy, Insert**" or "**Add**" a new entry. If you select "**Insert**" or "**Add**" a list of available directives/subdirectives/parameters pops up. Select an item an click **Okay**. Detailed description of the directives may be found in chapters describing every simulator below.

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The most convenient way of starting a new project is to select a proper existing project and then to click the "Copy" button. A new project will be created with "(copy)" at the name end in the "Name" window. Edit the name in the "Name" window and click the "Update" button. To modify directives/parameters switch to the "Parameter Settings" page as described above.

If you need to start a new project type a name of the project in the "Name" window, select method in the "Method" window and click the "Add" button. A project with default directive/parameter settings will be created. Change current page to "Project Settings" and edit parameters as described above.

To run a simulation click the "Run" button. After the simulation is complete you may display the results by clicking on "2D Output" or "3D Output" button for plotting I-V curves or 3D/contour plots of two-dimensional distributions respectively. Click on "Curve" or "Surface" for "2D Output" or "3D Output" respectively to plot an IV-curve or a surface.

2D distributions available for plotting are: electrostatic potential, carrier and current densities, Fermi quasi-potentials, electric field components, etc. You may also plot 2D cross-sections and IV-plots as well as transconductances as a function of applied voltage. For more information on Graphics Tools refer to Chapter 3 below.

MICROTEC USER INTERFACE

2.1. Introduction

MicroTec is a shell integrating four programs for silicon process-device simulation:

- SiDif- two-dimensional SImulator for DIFfusion and oxidation
- MergIC- program for MERGing fragments of IC elements
- SemSim- two-dimensional steady-state SEMiconductor device SIMulator
- SibGraf- interactive 3D and 2D graphics

MicroTec is a highly robust 2D semiconductor process-device simulation package which can be run on IBM PCs and compatibles with a reasonable CPU time and low memory requirements.

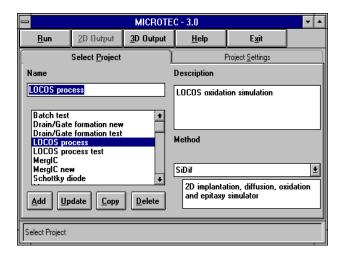
2.2. Running MicroTec

MicroTec main menu has two tabbed pages: 'Select Project' page' and 'Project Settings' page that can be switched by clicking on the respective tab.

Select Project page

The first page of the MicroTec main menu, called the 'Select Project' shown below comprises the following objects:

- Run Bar with 'Run', '2D Output', '3D Output', 'Help' and 'Exit' buttons.
- Edit Bar with 'Add', 'Update', 'Copy', and 'Delete' buttons.
- Name Text Box showing the current project name.
- Method Text Box showing the simulator used for the current project.
- **Project List Window** showing the list of available projects.
- **Project Description Window** with a brief description of the current project.
- Method Description Window with a brief description of the current project simulator.



To select a project in the project list window on the "Select Project" page, click the left mouse button at a project name. The corresponding project and simulator name will be appear in the "Name" and "Method" text box respectively.

If you need to change a project name or project description, edit the text in the respective window and click '**Update**' button.

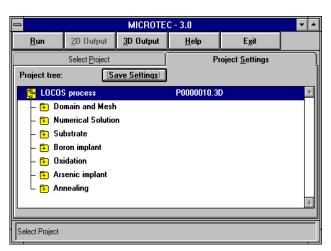
If you need to start a new project type a name of the project in the "Name" window, select a method in the "Method" text box and click the "Add" button. A project with default settings will be created. Change current page to the "Project Settings" page and edit parameters as described in Section "Project Settings page" on page 16.

Another way of starting a new project is to copy an existing project by clicking the "Copy" button and then to modify directives/parameters on the "Parameter Settings" page. A new project with '(copy)' at the name end will be created. To modify the project name, change the name in the "Name" text box and click the "Update" button in the main MicroTec window.

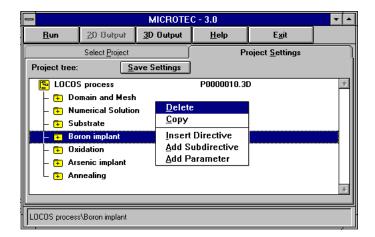
To run a simulation click the "Run" button. After the simulation is complete you may display the results by clicking on "2D Output" or "3D Output" button for plotting IV curves or 3D/contour plots of two-dimensional distributions of various variables such as electrostatic potential, carrier and current densities, Fermi quasi-potentials, electric field components, etc. See Section "Micro-Tec Graphics: SibGraf" on page 19 for more information on the MicroTec graphics.

Project Settings page

To modify project settings click on "**Project Settings**" tab. The other page of the main **MicroTec** menu will appear showing a **Project Tree** containing directives, subdirectives and parameters. Click the left mouse button on a folder symbol to open it. Double-click the left mouse button on a parameter to edit it.



To modify the tree structure, click a directive/subdirective/parameter by the left and then the right mouse button. A new window pops up allowing you to '**Delete**', '**Copy**', '**Insert**' or '**Add**' a new entry.



If you select 'Delete' the current entry will be deleted. If you select 'Copy' a new entry with a copy of the current entry content will be added at the end of the project tree. If you select 'Insert' or 'Add' a new window pops up showing you a list of entries available to add at this stage. Select one of them and click 'Okay'. Parameters that are added have default values. To change this value, double-click the parameter and a new window will pop up showing you the parameter current value and a brief parameter description. Edit the parameter value in the text box and click 'Okay'.

There are different types of directives in **MicroTec**: unique/non-unique and mandatory/optional. For example, '**IV** curve' subdirective is optional and non-unique, that is one may skip this subdirective or may use it a number of times to generate a family of IV curves. On contrary, the '**Basic**' directive is mandatory and unique. Any new created project will have all mandatory directives in it with the default values of parameters. Mandatory directives cannot be deleted.

Method Text Box

When you start a new project you may select appropriate **Method** in the **Method Text Box**. The following four options are available:

- SiDif- two-dimensional SImulation of implantation, diffusion and oxidation
- MergIC- program for MERGing fragments of simulated by SiDif
- **SemSim** two-dimensional steady-state semiconductor device simulation
- Batch- batch mode simulation of any number of process and/or device simulations

MICROTEC GRAPHICS: SIBGRAF

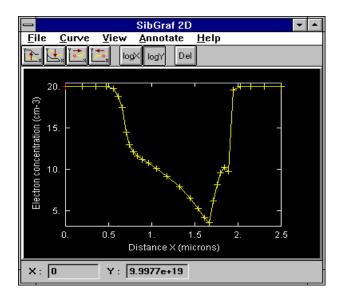
3.1. Introduction

SibGraf is a fast and user-friendly software tool for plotting I-V curves and two-dimensional distributions of the electrostatic potential, carrier and current densities, Fermi quasi-potentials, generation rate and electric field components. It is menu-driven and includes on-line help.

SibGraf generates 3D plots, contour lines, color maps, 2D cross-sections of 3D plots and 2D plots for I-V data.

3.2. SibGraf 2D Output

This function allows you to plot any column, or a product of any two columns, or a ratio of any two columns as a function of any column in the 2D data file. The 2D data file is generated by **SemSim** and represents IV data and transconductance data. When you click on "**2D Output**" button in the main **MicroTec** window, a new window pops up with five menu choices: **File, Curve, View, Annotate** and **Help**. The subtopics available under these menus are described below. To zoom a portion of the graph use the left muse button as described in section Zooming below. You may also use **Annotate** command which is also described below. The **Tool Bar** buttons allow you to change the current point and curve, switch to log scale and back and delete the current curve, shown in yellow color. More information is available in Section "2D Tool Bar" on page 23.



File

Open - Open a picture file previously created by this program.

Load - Load data from a file containing 2D data, e.g. IV curves.

Save - Save the plot to the picture file that is currently open. If there is no picture file that is currently open (if the **Load** function was used instead) then this function will behave as the 'Save As' function described below.

Save As - Save the plot to a picture file. A window will be provided to allow you to choose the file name.

Clear - Clear the plot window.

Print - Print the plot to a printer or to a Postscript file.

New Window - Open new **Sibgraf** 2D window.

Exit - Close the window.

Curve

Add - Open a window which displays the information about the current data file. A file must have been previously loaded with the '**Load**' command under the '**File**' submenu for this to work. A new window appears showing the information extracted from the data file which has been loaded. It enables the user to select curves to be shown in the plot window.

The first line of this window shows the current family number and name and allows the user to switch between families. Odd family numbers correspond to the IV data and even correspond to transconductance data. The table contains names as well as maximum and minimum values of each column in the current family. The first two check boxes beside each column allow the user to choose which column will be the X axis and which will be the Y axis. The third check box allows the user to choose a column which will be multiplied by the column chosen as the Y axis. In this case a product of the respective elements of the two columns will be plotted. The fourth check box allows the user to choose a column which will be used as a divider for the Y axis. In this case a ratio of the respective elements of the two columns will be plotted, e.g. current gain $\beta = I_C/I_B$.

The user can type the name of the curve being created into the box called 'Curve Name'. If no curve name is specified, it is the same as the name of the curve given as the column chosen as the Y axis. When all required information is selected (at least the X and Y axes must be given), the curve may be added to the plot by pressing the 'Add' button. The data used to create a curve may be viewed later by selecting the 'Source' item from the 'Curve' menu.

Copy - Copy the current curve from the plot to the **Sibgraf** clipboard. A very useful feature to create different windows with different sets of curves in each of them.

Paste - Add the curve from the **Sibgraf** clipboard to the current plot.

Delete - Delete the current (yellow) curve from the plot.

Source - Open a window which shows the data source for the current curve.

Line, Color, Marker - Change the corresponding attribute of the current curve.

View

Options - Open a window where the user can assign labels for horizontal and vertical axes and the title for the plot. The user can also specify the lowest value for the logarithm function corresponding to the argument approaching zero. The user can choose to show only markers or only lines for all curves in the current plot. Information in this window may be saved by pressing "**Save**" button. File "setup.mt" will be created and the settings will be read in every time a new **SibGraf** 2D window is opened.

Grid, Legend - Switch grid and legend on and off.

Zoom Out - Turn off zoom; can also be done with ESC key.

Annotaate

See general description of **Annotate** command in Section "Annotate" on page 28.

Help

Index - Help index for SibGraf.

About - Display SibGraf info.

2D Status Bar

The status bar is the strip at the bottom of the plot window. It shows the value of the X and Y coordinates for the current marker on the current curve. The current marker is shown in red color.

2D Tool Bar

The tool bar is the line of buttons just below the main menu and above the plot window. The first two buttons are used to change the current curve which is shown in yellow color. Each click will change the current curve to the next one. The first button cycles upward through the curves and the second cycles downward. This can also be done by using the up and down arrow keys on the keyboard.

The next two buttons change the current point marker on the current curve. The current marker is shown in red color. The buttons move the point to the left and right respectively. This can also be done using the left and right arrow keys on the keyboard.

The two buttons **Log X** and **Log Y** are used to switch to logarithmic scale and back on the X and Y axis respectively.

The last button, marked **Del**, deletes the current curve from the plot.

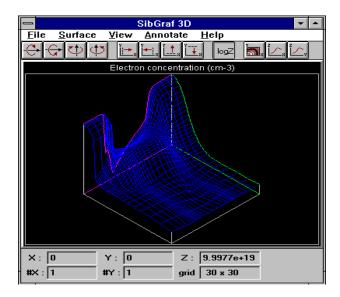
2D Data File Structure

This section describes the format of a data file that can be loaded by the '**Load**' selection under the **File** menu. By default the program looks for files with an extension of '.2d*', where * is any character.

Each data file contains sets of data, which are referred to as 'families'. Each family is a number of data columns each with the same number of entries (rows). After the file is loaded, the user may choose which column is the X axis and which column or columns will be shown on the Y axis. The user may also choose to plot a product or ratio of any two columns on the Y axis. It allows to plot such quantities as current gain $\beta = I_C/I_B$, etc.

3.3. SibGraf 3D Output

The user has five menu choices: 'File, Surface, View, Annotate' and 'Help'. The subtopics available under these menus are described below.



File

Open - Open a picture file previously created and saved by this program.

Load - Load data from a file containing 2D distribution data. By default the files should have extension *.3d*.

Save - Save the plot to the picture file that is currently open. If there is no picture file that is currently open (if the **Load** function was used instead) then this function will behave as the 'Save As' function described below.

Save As - Save the plot to a picture file. A window will be provided to allow you to choose the

picture file name.

Clear - Erase the plot that is currently in the plot window.

Print - Print the plot that is currently in the plot window to a printer or to a Postscript file.

New Window - Opens new Sibgraf 3D window.

Exit - Close the SibGraf 3D window.

Surface

Source - Opens a window which shows the data source for the current surface.

If the current plot was invoked through the Open function, "**Source**" is the only subitem under **Surface**. If the file with 2D distribution data was loaded through the '**Load**' function all the surfaces contained in that file are listed after the "**Source**" item. Any of these surfaces may be plotted.

View

Options - Opens a window where the user can assign labels for horizontal and vertical axes and the title for the plot. The user can also specify the lowest value for the logarithm function corresponding to the argument approaching zero.

Tool bar, Status bar - If checked, the items will be shown in the window. If you would like to increase the plotting area you may want to uncheck them. See the description below in this section.

Redraw - Redraw current surface.

Zoom Out - Turns off zoom; can also be done with ESC key.

Annotaate

See Help on 'Annotate' below in Section "Annotate" on page 28.

Help

Index - Open a window with the help index.

About - Display **SibGraf** info.

3D Status Bar

The status bar is the strip at the bottom of the plot window. The first line of three numbers in the

status bar shows the values of the X and Y coordinates for the corresponding current cross-sections and the Z value at the point of their intersection. The bottom line shows the mesh step numbers of current X and Y cross-sections and the overall dimension of the grid.

3D Tool Bar

The tool bar is the line of buttons just below the main menu and above the plot window.

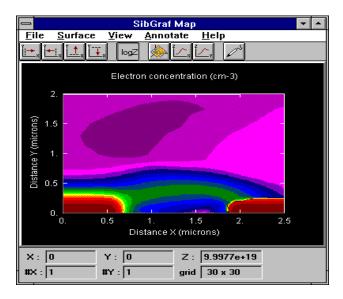
The first four buttons are used to rotate the surface about horizontal and vertical axes associated with the screen. The next four buttons are used to move the current X- and Y- cross-sections forward and backward. This can also be done by using the arrow keys on the keyboard.

The button 'Log Z' is used to switch to logarithmic scale and back.

The last three buttons are used to open **SibGraf Map** window with the same data and **SibGraf** 2D windows with the current X and Y cross-sections, or to add one more curve to the existing X or Y window.

3.4. SibGraf Map Menu

The user has five menu choices: 'File, Surface, View, Annotate' and 'Help'. The subtopics available under these menus are described below.



File

Open - Open a file containing a plot previously created and saved by this program.

Load - Load data from a file containing 2D distribution data.

Save - Save the plot to the picture file that is currently open. If there is no plot that is currently open (if the Load function was used instead) then this function will behave as the 'Save As' function described below.

Save As - Save the plot to a picture file. A window will be provided to allow you to choose the file name.

Clear - Erase the plot that is currently in the plot window.

Print - Print the plot that is currently in the plot window to a printer or to a Postscript file.

New Window - Open a new Sibgraf Map window.

Exit - Close the window.

Surface

Source - Opens a window which shows the data source for the current plot.

If the current plot was invoked through the 'Open' function, 'Source' is the only subitem under 'Surface'. If the file with 2D distribution data was loaded through the 'Load' function all surfaces contained in that file are listed after the item 'Source'. Any of these surfaces may be plotted.

View

Axis Limits - Opens a window where the user can assign ranges for horizontal and vertical axes.

Options - See Help on 2D Options in Section "View" on page 23.

Set Contours - see help on 'Map Set Contours' in Section "Map Set Contours" on page 28.

Rainbow8, Rainbow16, BlackWhite, Contours - each of these four items describes one of the possible four SibGraf Map representations: Map of 8 colors, Map of 16 colors, Map of 8 gray shades and Contour Map.

Grid, Legend - Show/hide discretization mesh and legend for **Color Map**.

Redraw - Redraw current plot.

Zoom Out - Turn off zoom; can also be done with ESC key.

Annotate - See Help on **Annotate** below in Section "Annotate" on page 28.

Help

Index - Open a window with the help index.

About - Displays SibGraf info.

Map Set Contours

'Set Contours' subitem under the 'View' menu item of the SibGraf Map opens the window where the user can assign the levels at which the contour lines are drawn for the current surface.

Automatic - the user can assign the start and the step values for Z (or Log Z) and choose whether all or none of the contour labels are shown.

Manual - the user can add a new contour line by pressing the 'Add' button and specifying Z (or Log Z) values for it, remove existing contour line by choosing it in the table and pressing the button **Remove**, or modify the existing contour lines by changing its Z (or Log Z) value. The check box in front of each level value indicates whether the contour labels for all contours at this level are shown or not.

The user can also modify the existing contour line and its label by positioning the mouse on a particular label on the plot and pressing the right mouse button. A menu will appear through which the user can choose to remove from the plot either this label or all contour lines at the corresponding level.

The location of a label can be changed by dragging the label with the left mouse button. If by this operation the label is moved completely out of the plot area it becomes invisible, although it still exists and will appear if, for example, the **Unzoom** function is used.

Map Status Bar

The status bar is the strip at the bottom of the plot window. If the probe mode is off the first line of three numbers in the status bar shows the values of the X and Y coordinates for the corresponding current sections and the Z value at the point of their intersection.

If the probe mode (see below) is on the first line of three numbers in the status bar shows the values of the X, Y and Z coordinates at the current mouse position. The bottom line shows the numbers of current X and Y sections and the overall dimension of the grid.

Map Tool Bar

The tool bar is the line of buttons just below the main menu and just above the plot window. The first four buttons are used to move the current X- and Y- sections forward and backward. This can also be done by using the arrows on the keyboard. The 'Log Z' button is used to switch to and from a logarithmic scale of the Z coordinate. The next three buttons are used to open SibGraf Map window with the same data and SibGraf 2D windows with the current X- and Y- sections. The last is the 'Probe' button, used to switch on and off the probe mode (see Help on Map Status Bar above).

3.5. Annotate

All of SibGraf 2D, 3D and Map windows have Annotate item in their main menu. Two types of

annotate objects can be created: **Line** and **Text**. Annotate objects are associated with the real X and Y coordinates and not with the window or screen position and, therefore, move with respect to the window when such operations as zooming or change of the size of the window are performed.

When the subitem **Line** is chosen, the user can draw a line consisting of a number of straight segments defining the start and end points of each segment by clicking with the left mouse button in the plot area. The click of the right mouse button will terminate the line drawing. To modify existing **Annotate Line** object first select it by clicking the left mouse button at the line. Then either the whole line or any of its nodes can be moved to the desired position with the left mouse button. Click with the left mouse button anywhere away from the line will terminate the modification mode.

When the subitem **Text** is chosen, a window will appear, where the user can type the required text and chose whether the border around the text is shown.

When the **OK** button is pressed the text will be placed in the centre of the plot area. To move the existing **Annotate Text** object first select it by clicking the left mouse button inside the text region. Then the text region can be moved to the desired position by dragging it with the left mouse button. If the content of the text object is to be changed, the user should chose subitem **Edit** under **Annotate** in the main menu. A click of the left mouse button anywhere away from the text region will terminate the modification mode. The user can delete an annotate line or text by selecting it as the current annotate object as described above and then choosing subitem **Delete** under **Annotate** in the main menu.

3.6. Zooming

The user may zoom in on a particular rectangle of any plot: **2D**, **3D** or **Map** as follows. Position the cursor over a point on the plot that you would like to use as the corner of a new plot. Press and hold the left mouse button as you move the mouse, which will show a rectangle on the plot corresponding to the area that will be shown on a new plot. When you have a rectangle defined that covers the area of the plot that you would like to zoom in on, release the mouse button and the plot will be replaced by a plot of the selected area. To restore the original plot you may press the **ESC** key or select '**Zoom Out**' from the '**View**' menu. In **SibGraf 2D** and **Map** windows you may unzoom the plot by selecting a rectangle outside the plotting area using the left mouse button.

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4.1. Introduction

It is well known that analytical approximations for doping profiles typically do not adequately reflect results of fabrication processing, especially for devices with submicron dimensions.

A program named **SiDif** has been developed [1] to compute two-dimensional impurity profiles of VLSI elements that have undergone various fabrication steps. The fabrication process may include processing steps such as ion implantation or surface deposition (arsenic, boron or phosphorous) with subsequent annealing under oxidizing or inert ambient. Resulting doping profiles may be used in a straightforward manner to generate the entire structure of a semiconductor device for subsequent evaluation of I-V curves in a few minutes on a PC.

The algorithm [2] is based on the finite-difference formulation and a rectangular mesh. The physical model adopted describes the diffusion process for up to three interacting charged impurities in a two-dimensional domain with moving oxide boundary and impurity segregation at the Si/SiO_2 interface. In the case of implantation the initial profiles of each impurity are approximated by the conventional Runge's model [12].

The program is written in FORTRAN-77 and can be used on IBM-AT/386 or higher with an EGA/VGA/SVGA adapter running under Windows. Dynamic memory allocation is used in **SiDif** with 400 Kbytes required for a 2500 node mesh. Typical process simulation requires about a minute on Pentium-100.

4.2. Physical model

Diffusion of charged impurities is influenced by the presence of an internal electric field. The physical model for diffusivities which accounts for the influence of charged defects is taken from [4-5].

$$J_k = D_k \nabla C_k + q Z_k \mu_k C_k E \tag{4.1}$$

where C_k is the concentration of the k-th impurity, D_k is the diffusivity, Z_k is the charge number, μ_k is the electrical mobility, q is the elementary charge and E is the electric field. This model uses the quasineutral approximation, which relates the electric field to impurity concentrations:

$$E = -\nabla \Psi = -\frac{kT}{q} \nabla \ln \left(\frac{n}{n_i} \right) \tag{4.2}$$

where

$$n = -\frac{1}{2} \left(\sum_{k} Z_{k} C_{k} + \sqrt{\left(\sum_{k} Z_{k} C_{k}\right)^{2} + 4n_{i}} \right)$$
 (4.3)

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Here n is the electron concentration and n_i is the intrinsic carrier concentration

$$n_i = n_{i0} T^{\varsigma} \exp\left(\frac{-E_G}{2kT}\right). \tag{4.4}$$

From (2) and (3) we obtain

$$E = -\frac{kT/q}{\sqrt{\left(\sum_{k} Z_{k} C_{k}\right)^{2} + 4n_{i}}} \sum_{k} Z_{k} \nabla C_{k}.$$

$$(4.5)$$

Assuming that the Einstein relation $\mu_k = \frac{Z_k q}{kT} D_k$ is valid, the diffusion equation transforms to

$$J_{i} = D_{i} \left(\nabla C_{i} + Z_{i} C_{i} \frac{\sum_{k} Z_{k} \nabla C_{k}}{\sqrt{\left(\sum_{k} Z_{k} C_{k}\right)^{2} + 4n_{i}}} \right)$$

$$(4.6)$$

In the case of one impurity the drift can be taken into account by introducing a multiplicative factor for the diffusivity [3] but for several impurities the following system of coupled equations must be solved.

$$\frac{\partial C_i}{\partial t} = \nabla \left(D_i \nabla C_i + D_i Z_i C_i \frac{\sum_k Z_k \nabla C_k}{\sqrt{\left(\sum_k Z_k C_k\right)^2 + 4n_i}} \right). \tag{4.7}$$

Diffusion coefficient

The diffusivity of arsenic and boron, accounting for single charged defect influence, is chosen in the form [3,4,5]

$$D_k = D_{0k} \exp\left(\frac{-E_{0k}}{kT}\right) \left(\frac{1+\beta_k \eta}{1+\beta_k}\right) \tag{4.8}$$

where $\eta = \frac{n}{n_i}$ for arsenic, $\eta = \frac{p}{n_i}$ for boron, D_{0k} and E_{0k} are the intrinsic diffusion coefficient

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and activation energy of the k-th impurity respectively. The parameter β_k defaults to 3 for boron and 100 for arsenic.

The phosphorus diffusivity was chosen as in [5,6] and accounts for the diffusion via neutral, and single and double negatively charged vacancies.

$$D_P = D_0 \exp\left(\frac{-E_0}{kT}\right) + D_1\left(\frac{n}{n_i}\right) \exp\left(\frac{-E_1}{kT}\right) + D_2\left(\frac{n}{n_i}\right)^2 \exp\left(\frac{-E_2}{kT}\right)$$
(4.9)

Oxidation enhanced diffusion

The diffusivity during oxidation is modified depending on the rate of oxidation, in order to describe the oxidation-enhanced (or oxidation-retarded) diffusion [8]. Oxidation changes the diffusivity because it generates interstitials in the crystalline lattice. In **SiDif** the Taniguchi model is used [8]

$$D_i^{ox} = D_i + \Delta D_i \left(\frac{dU}{dt}\right)^{\beta_{ox}} \exp\left(\frac{-E_{ox}}{kT}\right) \exp\left(\frac{-\Delta x}{\lambda_x}\right) \exp\left(\frac{-y}{\lambda_y}\right) . \tag{4.10}$$

The diffusivity enhancement decays exponentially in the above formula where Δx is the distance from the mask edge (Δx =0 outside the masked region) and y is the vertical distance from the interface [8].

Analytical oxidation model

For the analytical oxidation model the Deal-Grove formulation is used [7] in SiDif

$$\frac{dU}{dt} = \frac{B}{2U + A} \tag{4.11}$$

where U is the oxide thickness and A, B are kinetic constants which are proportional to the pressure and depend on the ambient composition. The values A, B are significantly higher if the ambient contains water vapor or HCl. In the latter case the constants are given by [16,17]

$$B = P_{ox}B_{o}\exp\left(\frac{-E_{B}}{kT}\right), \quad \frac{B}{A} = OR_{ox}P_{eff}R_{o}\exp\left(\frac{-E_{R}}{kT}\right). \tag{4.12}$$

Here P_{ox} is the pressure of the oxidizing ambient in atmospheres and P_{eff} is the effective pres-

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sure for the linear kinetic coefficient $\frac{B}{A}$. In the case of wet oxidation $P_{eff} = P_{ox}$ and in the case of dry oxidation $P_{eff} = P_{ox}^{\beta_p}$. The factor OR_{ox} depends on the silicon orientation [17].

If there is an initial oxide film with a thickness of U_o on the surface of the semiconductor then (4.11) leads to

$$U(t) = \sqrt{\left(U_0 + \frac{A}{2}\right)^2 + Bt} - \frac{A}{2}$$
 (4.13)

Usually only a fragment of the wafer surface is exposed to the oxidizing ambient while the rest of the surface is covered by a nitride mask. In this case oxidation in the area near the mask edge is described by the "bird's beak" formula

$$U(x,t) = U_0 + \frac{U(t) - U_0}{2} erf\left(\frac{x - xm - \delta}{\gamma}\right)$$
(4.14)

with the following empirical parameters [10]

$$\delta = \frac{\delta_0 - \delta_1 T + \delta_1 \ln(U_0)}{1 + 3\chi} + (\delta_2 - \delta_3 T - \delta_4 \chi) U(t)$$
(4.15)

$$\gamma = \frac{\gamma_0 - \gamma_1 T + \gamma_1 \ln(U_0)}{1 + 3\chi} + (\gamma_2 - \gamma_3 T - \gamma_4 \chi) U(t)$$
(4.16)

where $\chi = 1$ and 0 for (111) and (100) orientation respectively.

Segregation

The oxidation of silicon is accompanied by the segregation, in other words, a jump in the impurity concentration at the moving Si/SiO_2 interface. The segregation causes an impurity flux density at the interface which may be written as

$$J_{ox} = C_b \left(1 - \frac{1}{\alpha_s m} \right) v_{ox} \tag{4.17}$$

where C_b is the impurity concentration in Si at the SiO₂ boundary, m is the segregation coefficient, v_{ox} is the oxide growth rate in the direction normal to the interface and α is the ratio of volumes of Si and SiO₂ that is equal to 0.44.

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For boron

$$m = A_{seg} \exp\left(\frac{-E_{seg}}{kT}\right), \ \lambda = A_{\lambda} \exp\left(\frac{-E_{\lambda}}{kT}\right).$$
 (4.18)

For phosphorous and arsenic the segregation coefficient is large (about 100) and usually close to the equilibrium value [11] so that the impurity may be considered to be completely pushed into the silicon. In this case

$$J_{ox} = C_b v_{ox} (4.19)$$

At high oxidation rates the segregation may cause concentrations at both sides of the interface to not reach equilibrium values. In this case a correction was proposed [10]

$$J_{ox} = C_b \left(1 - \frac{1}{\alpha_s m} \right) \frac{v_{ox} \lambda}{\lambda + v_{ox}}$$
 (4.20)

where λ is the kinetic constant of the segregation reaction. Equilibrium values of m were taken from [9].

Ion implantation

Ion implantation is widely used now as a standard tool for the doping of semiconductor wafers. In **SiDif** an analytic ion implantation model is employed.

In a one dimensional case the implant is described by a Gaussian distribution

$$I(y) = \frac{1}{\sqrt{2\pi}\sigma_y} \exp\left(\frac{-(y - R_p)}{2\sigma_y^2}\right)$$
 (4.21)

where R_p and σ_y are the projected range and vertical standard deviation respectively, and y is the distance from the top of the wafer material.

The two-dimensional implant profile is described by the formula[15]

$$I(x,y) = \frac{I(y)}{2} \left(erf\left(\frac{x - x_r}{\sqrt{2}\sigma_x}\right) - erf\left(\frac{x - x_l}{\sqrt{2}\sigma_x}\right) \right)$$
(4.22)

where x_r and x_l are the coordinates of the left and the right edges of the grid cell. To obtain the

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final implant distribution, expression (4.22) is integrated over the exposed surface of the wafer.

4.3. Simulation algorithm

The finite-difference technique [2] was chosen for the diffusion equation discretization due to a property of the matrix equation to be solved (symmetrical 5-diagonal matrix with diagonal dominance). For each mesh node the difference mass balance equation is written. For nodes adjacent to an oxide boundary the segregation flux of an impurity caused by oxide motion is included [2]. The total impurity dose within the semiconductor and oxide is conserved to the extent of the floating point accuracy of the computer.

For the solution of several coupled diffusion equations the finite-difference equations of each impurity are solved sequentially, with initial values of impurity concentrations taken from the previous iteration or previous time step. Iterations continue until the solution for all impurities converges to a given accuracy. The incomplete factorization method [13] combined with the conjugate gradient method [14] are employed to solve the equations of the 5-diagonal matrix.

The algorithm was tested by comparing results with examples published in papers [3,5,6,10]. The following example of LOCOS process simulation demonstrates CPU time requirements [2].

The boron is implanted with 100 KeV energy and a 10^{14} ions/cm² dose and the arsenic is implanted with 100 KeV and a 10^{15} ions/cm² dose. An annealing step at 1000 C in a wet ambient follows for 30 minutes. Ten minutes of CPU time were required for this example using a mesh of (45x45) nodes on a 25 MHz PC-386. The same CPU time on a 12 MHz PC-AT/286 was required for the simulation with a mesh of (25x25) and twice as large time step.

The difference in position of the contour lines for both calculations was less than 0.01 microns in the region of the p-n junction. In the regions with concentration values of 10^{14} - 10^{15} cm⁻³ the difference was 0.02 - 0.03 microns. Thus the important parameter, p-n junction depth, is determined with an accuracy sufficiently high [2] for an I-V curve evaluation.

4.4. References

- [1] M.S.Obrecht, A.L.Alexandrov, "SIDIF a program for two-dimensional modelling of diffusion and oxidation," Solid-State Electronics, Software Survey Section, v.34, No 8, 1991
- [2] A.L.Alexandrov, M.S.Obrecht, G.V.Gadiyak, "Efficient finite-difference method for numerical modelling of thermal redistribution of interacting impurities under oxidizing ambient", Solid State Electronics, v.35, p.1549-1552, 1992
- [3] "Process and Device Simulation for MOS-VLSI Circuits," Ed.by P.Antognetti, R.W.Dutton et al., Martinus Nijhoff Publishers, 1983.
- [4] R.W.Dutton and D.A.Antoniadis, "Models for computer simulation of complete IC fabrica-

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- tion processes," IEEE Trans. Electr. Dev., v.ED-26, p.490.1979.
- [5] C.D.Maldonado, "ROMANS II A two-dimensional process simulator," Appl.Phys., vol. A31, p.119, 1983.
- [6] R.W. Dutton, C.P. Ho et al. "VLSI process modelling SUPREM III," IEEE Trans. Electr. Dev., v.ED-30, p.1439, 1983.
- [7] B.E. Deal and A.S. Grove, "General relationship for the thermal oxidation of silicon", J. Applied Physics, vol. 36, p. 3770, 1965.
- [8] K.Tanigushi et al. "Two-dimensional computer simulation models for MOS-LSI fabrication processes," IEEE Trans.Electr.Dev., v.ED-28, p.574,1981
- [9] R.B. Fair and J.C. Tsai, "Theory and measurement of boron segregation in SiO₂ during oxidation", J. Electrochem. Soc., vol. 125, p. 2050, 1978.
- [10] V.I.Koldyaev, V.A.Moroz et al. "Two-dimensional simulation of the doping and oxidation of silicon". Optoelectronics, Instrumentation and Data Processing (Avtometria), No.3, p.50,1988.
- [11] A.S. Grove et al, "Redistribution of acceptor and donor impurities under oxidation of silicon", J. Applied Physics, vol. 35, p. 2695, 1964.
- [12] H.Runge "Distribution of implanted ions under arbitrarily shaped mask," Phys. Stat. Sol., v.39(a), p.595,1977
- [13] G.Schneider, M.Zedan. "A modified strongly implicit procedure for the numerical solution of field problem," Numerical Heat Transfer, vol.4, p.1, 1981.
- [14] H. A. Van Der Vorst, "Bi-CGSTAB: a fast and smoothly converging variant of Bi-CG for the solution of nonsymmetric linear systems," SIAM Journ. Sci. Stat. Comput., vol. 13, pp. 631-644, March 1992.
- [15] S. Furukawa, H. Matsumura and H. Ishiwara,. "Theoretical Considerations on Lateral Spread of Implanted Ions," Jap. J. Apll. Phys., vol. 11, No. 2, pp. 134-142, 1972.
- [16] L.N. Lie, R.R. Razouk and B.E. Deal, "High Pressure Oxidation of Silicon in Dry Oxygen", J. Electrochem. Soc., vol. 129, No. 12, pp. 2828-2834, 1982.
- [17] R.R. Razouk, L.N. Lie and B.E. Deal, "Kinetics of High Pressure Oxidation of Silicon in Pyrogenic Steam", J. Electrochem. Soc., vol. 128, No. 10, pp. 2214-2220, 1981.

4.5. Running SiDif

To run **SiDif** from the **MicroTec** shell, select a **SiDif** project in the project list on the "**Select Project**" page and click "**Run**" in the main **MicroTec** menu. You may also "**Add**, **Update**, **Copy**" and/or "**Delete**" projects in the main menu.

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If you want to modify a project, click on "**Copy**" button. A new project will be created with the old project name and "(copy)" at the end. After that you may change the project settings by clicking on the "**Project Settings**" page tag. This will display directives in the input file. Double click on a directive unfolds it and lets you edit the parameters.

If you want to start a new project, type the project name in the "Name" window, select SiDif in the "Method" window and click "Add". A new project will be created with default parameter settings.

On the output **SiDif** generates a doping data file which may be directly used in the device simulation. This output file also may be used by **MergIC** to produce a more complex final device structure by copying, overlaying and symmetrizing fragments simulated by **SiDif**.

Black "**3D Output**" button means that the result has been successfully computed and you may plot the output doping profiles by clicking on this button. If it is grey, click "**Run**" button to perform process simulation and after the result has been computed the button becomes black.

4.6. SiDif input file

SiDif main input file contains directives and parameters. Each directive starts a group of parameters, separated by spaces or commas and ended by ';'. The computational domain and the mesh are the same for all the processing steps. The last step must be ended by \$. All directives after \$ will be ignored.

Note: Only one step with the oxidizing annealing is allowed in the present version of **SiDif**. Only implantation, deposition and inert annealing may be simulated after the oxide formation.

All the directives are of two types: basic directives and model parameter directives:

SiDif basic directives:

•MESH: computational domain and mesh parameters

•SUBS: substrate parameters

•SOLV: numerical solution control

•**PHDE**: phosphorus deposition

•BODE: boron deposition

•ASDE: arsenic deposition

•PHIM: phosphorus implant

•BOIM: boron implant

•ASIM: arsenic implant

•OXID: oxidation parameters

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•ANNE: annealing parameters

•EPIT: epi-layer formation

SiDif model parameter directives:

•BAND: Bandgap and intrinsic carrier concentration

•**DIFF**: Diffusivity of Arsenic, Boron and Phosphorus

•OED: Oxidation-enhanced diffusion

•DROX: Dry oxidation kinetic constants

•WEOX: Wet oxidation kinetic constants

•LOCO: Local oxidation "bird's beak" formula parameters

•SEGR: Segregation parameters

A description of the **SiDif** directives follows.

4.7. SiDif basic directives

MESH: computational domain and mesh parameters

Name	Default	Units	Description	
NX	30	none	Number of mesh nodes in X-direction (along the surface). It must be greater than 3.	
NY	30	none	Number of mesh nodes in Y-direction (into the depth of the domain). It must be greater than 3. A greater number of mesh nodes gives a higher computational accuracy at the expense of a larger CPU time.	
XX	1	um	Domain size in X-direction, microns. The domain should cover a region near edges of all the masks where the two-dimensionality takes place.	
YY	1	um	Domain size in Y-direction, microns. The domain should be deep enough to cover the maximum expected depth of the implanted or deposited dopant penetration.	
IM	1	none	This key must be 1 for a uniform mesh. If it is zero or negative, the mesh will be exponentially condensed in the origin of coordinates.	

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Name	Default	Units	Description
AX	0	none	Logarithm of the ratio of two adjacent mesh step sizes in the X-direction (if the mesh is not uniform).
AY	0	none	Analogous parameter for the Y-direction. Parameters AX, AY may be omitted if IM=1. Nonuniform mesh is preferable for a simulation including relatively fine structures near the surface.
COMM	'Comm'	none	Comment line.

SUBS: substrate parameters

Name	Default	Units	Description	
PH	1.0.1012	cm ⁻³	Initial uniform phosphorus concentration.	
ВО	1.0.1012	cm ⁻³	The same parameter for boron doping.	
AS	1.0.1012	cm ⁻³	The same parameter for arsenic doping.	
OR	100	none	Lattice orientation	
COMM	'Comm'	none	Comment line.	

SOLV: numerical solution control

Name	Default	Units	Description	
IB	1	none	Batch mode switch: If IB=1 (the default) then run without plotting after each processing step (batch mode).	
IT	100	none	Maximum number of iterations for the linear solver.	
RS	10-12	none	Residual convergence criterion for the linear solver.	
RL	10-3	none	Relative residual criterion for the linear solver.	
СО	10 ¹²	cm ⁻³	Value of the impurity concentration considered to be a background	
COMM	'Comm'	none	Comment line.	

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PHDE: phosphorus deposition

Name	Default	Units	Description	
XD	1	um	Position of the mask edge for a surface deposition of the dopant. In this case the surface acts as source with a constant concentration. The predeposition occurs in the surface region from 0 to XD (if XD is positive) or from XD to XX (if XD is negative). If XD is 0 or omitted, there is no predeposition. If XD is larger then XX, the dopant is deposited throughout the fragment surface	
CS	10 ¹⁹	cm ⁻³	Surface concentration of the dopant for the deposition. May be omitted if XD is omitted.	
COMM	'Comm'	none	Comment line.	

BODE: boron deposition

The same parameters are used as in the directive PHDE

ASDE: arsenic deposition

The same parameters are used as in the directive PHDE

PHIM: phosphorus implant

Name	Default	Units	Description	
XM	1	um	Position of the implantation mask edge. The dopant is implanted through the window from 0 to XM, if XM is positive and from ABS(XM) to XX if XM is negative. For uniform implantation all over the domain XM should be much greater then XX. Make it 0 or omit it to suppress the implantation	
DZ	10 ¹²	cm ⁻²	Implantation dose, (ignored if $XM = 0$)	
EN	40	KeV	Implantation energy, (up to 1000)	
COMM	'Comm'	none	Comment line.	

BOIM: boron implant

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The same parameters are used as in the directive **PHIM**

ASIM: arsenic implant

The same parameters are used as in the directive **PHIM**

OXID: oxidation parameters

Name	Default	Units	Description	
TC	1000	°C	Temperature of oxidation (centigrade).	
TM	1000	S	Time of oxidation in seconds.	
TAU	100	S	Initial time step in seconds. The recommended value is 30 s for a temperature of 1200 °C, 100 s for 1100 °C, 200 s for 1000 °C, and 500 s for 900 °C and lower. For an accurate evaluation on a fine mesh the recommended value is 2-10 times lower than the one above. Use a smaller TAU if the number of nonlinear iterations exceeds 7.	
OX	1	none	Type of annealing atmosphere: 1: dry oxygen, 2: wet ambient	
POX	1	Atm	Pressure of the oxidizing ambient (oxygen or vapor).	
XO	0	um	Position of the oxidation mask. The oxide grows in the region from 0 to XO if XO is positive and from XO to XX if XO is negative. To get a uniform oxide make XO a few times greater than XX.	
U0	0.001	um	Initial uniform oxide thickness (microns). It affects the rate of the oxide growth.	
COMM	'Comm'	none	Comment line.	

ANNE: annealing parameters

Name	Default	Units	Description	
TC	1000	°C	Temperature of annealing (centigrade).	
TM	1000	S	Time of annealing in seconds.	

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Name	Default	Units	Description
TAU	100	S	Initial time step in seconds. The recommended value is 30 s for a temperature of 1200 °C, 100 s for 1100 °C, 200 s for 1000 °C, and 500 s for 900 °C and lower. For an accurate evaluation on a fine mesh the recommended value is 2-10 times lower than the one above. Use a smaller TAU if the number of nonlinear iterations exceeds 7.
COMM	'Comm'	none	Comment line.

EPIT: epi-layer formation

Name	Default	Units	Description	
TC	1000	°C	Temperature of oxidation (centigrade).	
TM	2000	S	Time of oxidation in seconds.	
TAU	1	s	Initial time step in seconds. The recommended value is 30 s for a temperature of 1200 °C, 100 s for 1100 °C, 200 s for 1000 °C, and 500 s for 900 °C and lower. For an accurate evaluation on a fine mesh the recommended value is 2-10 times lower than the one above. Use a smaller TAU if the number of nonlinear iterations exceeds 7.	
PH	1.0.1012	cm ⁻³	Initial uniform phosphorus concentration.	
ВО	1.0·10 ¹²	cm ⁻³	The same parameter for boron doping.	
AS	1.0.1012	cm ⁻³	The same parameter for arsenic doping.	
TH	1	um	Thickness of the grown epitaxial layer. Existing profile of dopants is shifted by TH towards the depth of the domain and the dopant thermal redistribution during epitaxy is evaluated. Make sure that YY is large enough not to lose the buried layer.	
COMM	'Comm'	none	Comment line.	

4.8. SiDif model parameter directives

BAND: Bandgap and intrinsic carrier concentration

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$$n_i = n_{i0} T^{\varsigma} \exp\left(\frac{-E_G}{2kT}\right).$$

Symbol	Name	Default	Units	Description
n_{i0}	CINT	3.873·10 ¹⁶	cm ⁻³	Pre-exponential constant for intrinsic concentration
ς	EINT	1.5	none	Temperature exponent for intrinsic concentration
E_G	EGAP	0.60474	eV	Bandgap width for intrinsic concentration

DIFF: Diffusivity of Arsenic, Boron and Phosphorus

$$D_k = D_{0k} \exp\left(\frac{-E_{0k}}{kT}\right) \left(\frac{1 + \beta_k \eta}{1 + \beta_k}\right)$$

$$D_P = D_0 \exp\left(\frac{-E_0}{kT}\right) + D_1\left(\frac{n}{n_i}\right) \exp\left(\frac{-E_1}{kT}\right) + D_2\left(\frac{n}{n_i}\right)^2 \exp\left(\frac{-E_2}{kT}\right)$$

Symbol	Name	Default	Units	Description
D_{0k}	DX0A	22.9	cm ² /s	The pre-exponential constant for Arsenic
E_{0k}	DXEA	4.1	eV	The activation energy for Arsenic
β_k	BETA	100.	none	The charged vacancy effectiveness for Arsenic
D_{0k}	DX0B	0.555	cm ² /s	The pre-exponential constant for Boron
E_{0k}	DXEB	3.42	eV	The activation energy for Boron
β_k	ВЕТВ	3.0	none	The charged vacancy effectiveness for Boron
D_0	DX0P	3.85	cm ² /s	The pre-exponential constant for Phosphorous
E_0	DXEP	3.66	eV	The activation energy for Phosphorous
D_1	DMP	4.4	cm ² /s	The pre-exponential constant for Phosphorous
E_1	DMEP	4.0	eV	The activation energy for Phosphorous

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Symbol	Name	Default	Units	Description
D_2	DMMP	44.2	cm ² /s	The pre-exponential constant for Phosphorous
E_2	DMMEP	4.37	eV	The activation energy for Phosphorous

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OED: Oxidation-enhanced diffusion

$$D_i^{ox} = D_i + \Delta D_i \left(\frac{dU}{dt}\right)^{\beta_{ox}} \exp\left(\frac{-E_{ox}}{kT}\right) \exp\left(\frac{-\Delta x}{\lambda_x}\right) \exp\left(\frac{-y}{\lambda_y}\right) .$$

Symbol	Name	Default	Units	Description
ΔD_i	OEA0	0.0	cm ² /s	The OED for Arsenic (100) orientation
ΔD_i	OEA1	0.0	cm ² /s	The OED for Arsenic (111) orientation
ΔD_i	OEB0	1.66·10 ⁻⁵	cm ² /s	The OED for Boron (100) orientation
ΔD_i	OEB1	6.11e-6	cm ² /s	The OED for Boron (111) orientation
ΔD_i	OEP0	1.44·10 ⁻⁵	cm ² /s	The OED for Phosphorous (100) orientation
ΔD_i	OEP1	5.65·10 ⁻⁶	cm ² /s	The OED for Phosphorous (111) orientation
E_{ox}	OEE	2.08	eV	The activation energy for OED
λ_y	OELDY	25.0	um	The vertical coordinate exponent for OED
λ_y	OELDX	2.0	um	The lateral coordinate exponent for OED
β_{ox}	OEBOX	0.3	none	The oxidation rate exponent for OED

Deal-Grove oxidation kinetic constants

$$\frac{dU}{dt} = \frac{B}{2U+A}, B = P_{ox}B_o \exp\left(\frac{-E_B}{kT}\right), \frac{B}{A} = OR_{ox}P_{eff}R_o \exp\left(\frac{-E_R}{kT}\right), P_{eff} = P_{ox}^{\beta_p}.$$

DROX: Dry oxidation kinetic constants

Symbol	Name	Default	Units	Description
B_o	BD	0.214	um ² /s	Parabolic oxidation rate constant in dry O ₂
R_o	BAD	1730	um2/s	Linear oxidation rate constant in dry O ₂
E_B	BDE	1.23	eV	Parabolic activation energy in dry O ₂

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Symbol	Name	Default	Units	Description
E_R	BADE	2.0	eV	Linear oxidation activation energy in dry O ₂
β_p	BPF	0.75	none	Exponent of the effective pressure

WEOX: Wet oxidation kinetic constants

Symbol	Name	Default	Units	Description
OR_{ox}	OR0	0.595	none	Orientation coefficient for (100)
OR_{ox}	OR1	1.0	none	Orientation coefficient for (111)
T_c	TCP	950.0	°C	Parabolic constant critical temperature for wet O ₂
B_o	BW1	4.722	um ² /s	Parabolic oxidation rate constant in wet O_2 for $T < T_c$
E_B	BWE1	1.17	eV	Parabolic activation energy in wet O_2 for $T < T_c$
B_o	BW2	0.1167	um ² /s	Parabolic oxidation rate constant in wet O_2 for $T > T_c$
E_B	BWE2	0.78	eV	Parabolic activation energy in wet O_2 for $T > T_c$
T_c	TCL	900.0	°C	Linear constant critical temperature for wet O ₂
R_o	BAW1	575.0	um ² /s	Linear oxidation rate constant in wet O_2 for $T < T_c$
E_R	BAWE1	1.6	eV	Linear oxidation activation energy in wet O_2 for $T < T_c$
R_o	BAW2	4.917·10 ⁴	um ² /s	Linear oxidation rate constant in wet O_2 for $T > T_c$
E_R	BAWE2	2.05	eV	Linear oxidation activation energy in wet O_2 for $T > T_c$

LOCO: Local oxidation "bird's beak" formula parameters

$$U(x, t) = U_0 + \frac{U(t) - U_0}{2} erf\left(\frac{x - xm - \delta}{\gamma}\right)$$

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$$\delta = \frac{\delta_0 - \delta_1 T + \delta_2 \ln(U_0)}{1 + 3\chi} + (\delta_3 - \delta_4 T - \delta_5 \chi) U(t)$$

$$\gamma = \frac{\gamma_0 - \gamma_1 T + \gamma_2 \ln(U_0)}{1 + 3\chi} + (\gamma_3 - \gamma_4 T - \gamma_5 \chi) U(t)$$

Symbol	Name	Default	Units	Description
χ	KHI0	0.0	um	The Kappa for (100) orientation for bird's beak
χ	KHI1	1.0	um	The Kappa for (111) orientation for bird's beak
δ_0	DEL0	0.97	um	The first coefficient in Delta for bird's beak
δ_1	DEL1	6.0e-4	um	The second coefficient in Delta for bird's beak
δ_2	DEL2	0.034	um	The third coefficient in Delta for bird's beak
δ_3	DEL3	0.49	um	The forth coefficient in Delta for bird's beak
δ_4	DEL4	2.1e-4	um	The fifth coefficient in Delta for bird's beak
δ_5	DEL5	0.03	um	The sixth coefficient in Delta for bird's beak
γ_0	GAM0	0.83	um	The first coefficient in Gamma for bird's beak
γ_1	GAM1	4.5e-4	um	The second coefficient in Gamma for bird's beak
γ_2	GAM2	0.039	um	The third coefficient in Gamma for bird's beak
γ_3	GAM3	0.76	um	The forth coefficient in Gamma for bird's beak
γ_4	GAM4	3.5e-4	um	The fifth coefficient in Gamma for bird's beak
γ_5	GAM5	0.03	um	The sixth coefficient in Gamma for bird's beak

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SEGR: Segregation parameters

$$J_{ox} = C_b \left(1 - \frac{1}{\alpha_s m} \right) \frac{v_{ox} \lambda}{\lambda + v_{ox}}, \ m = A_{seg} \exp\left(\frac{-E_{seg}}{kT} \right), \ \lambda = A_{\lambda} \exp\left(\frac{-E_{\lambda}}{kT} \right)$$

Symbol	Name	Default	Units	Description
A_{seg}	SEGA	1.0.10 ²²	none	The Segregation coefficient for Arsenic
A_{seg}	SEGP	1.0.10 ²²	none	The Segregation coefficient for Phosphorous
A_{seg}	SGBD	13.4	none	The Segregation coefficient for Boron in dry O_2
E_{seg}	SBDE	0.33	eV	The Segregation activation energy in dry O ₂
A_{seg}	SBW0	65.2	none	The Segregation coefficient for Boron in wet O_2 for orientation (100)
A_{seg}	SBW1	104	none	The Segregation coefficient for Boron in wet O_2 for orientation (111)
E_{seg}	SBWE	0.66	eV	The Segregation activation energy in wet O ₂
A_{λ}	ALAM	1.25·10 ⁴	um/s	Pre-factor in critical oxidation rate in segregation for Boron
E_{λ}	ELAM	2.0	eV	Activation energy in critical oxidation rate in segregation for Boron

4.9. Examples of SiDif input files

A few examples of typical processing runs are presented in this section.

MOSFET fragment

Substrate with orientation <111> is doped initially with boron at 10^{15} cm⁻³. Boron is implanted at 60 KeV and $6\cdot10^{11}$ ions/cm² in the whole region and then arsenic is implanted at 100 KeV and 10^{15} ions/cm² through the mask and annealed at 1000 °C for 60 minutes in an inert ambient.

MESH:NX=20,NY=20,XX=1.,YY=0.7,IM=1, COMM='MOSFET';

SUBS:PH=1E12,BO=1E15,AS=1E12,OR=111;

BOIM:XM=2. DZ=6.E+11 EN=60;

ASIM:XM=-0.5 DZ=1.E15 EN=100;

ANNE:TC=1000,TM=3600,TA=600 OX=0;\$

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LDD MOSFET fragment

Boron and arsenic are implanted as in the above example into the same substrate. Then the mask is shifted by 0.35 microns and LDD arsenic is implanted at 100 KeV and 10^{12} ions/cm². Finally the wafer is annealed at $1000 \,^{\circ}\text{C}$ for $60 \,^{\circ}\text{C}$ minutes.

```
MESH:NX=20,NY=20,XX=1.,YY=0.7,IM=1, COMM='LDD MOSFET ';
SUBS:PH=1E12,BO=1E15,AS=1E12,OR=111;
BOIM:XM=2. DZ=6.E+11 EN=60;
ASIM:XM=-0.6 DZ=1.E15 EN=100;
ASIM:XM=-0.25 DZ=1.E12 EN=100;
ANNE:TC=1000,TM=3600,TA=600 OX=0;$
```

Fragment with LOCOS

Substrate is initially doped by boron at 10^{15} cm⁻³. Arsenic is implanted at 200 KeV and 10^{15} ions/cm² in the left side of the region. Then boron is implanted at 200 KeV and 10^{14} ions/cm² through another mask in the right side of the region. Annealing follows at 1100 °C for 1 hour in a wet oxidizing ambient to create a LOCOS structure.

```
MESH:NX=25,NY=35,XX=2,YY=2,IM=1, COMM='LOCOS';
SUBS:PH=1E12,BO=1E15,AS=1E12,OR=111;
ASIM:XM=1,EN=200. DZ=1E15;
BOIM:XM=-1,EN=100. DZ=1.E13;
ANNE:TC=1100,TM=3600,TA=100,OX=2,XO=-1,PO=0.9;$
```

Doping by deposition

The substrate is initially doped with phosphorus at 10^{15} cm⁻³. Then boron is deposited on the whole surface with a surface concentration of 10^{18} cm⁻³ for 30 minutes at 1000 °C. After this arsenic is deposited through the mask on the left side of the region with a surface concentration of 10^{20} cm⁻³ for 30 minutes at 1100 °C.

```
MESH:NX=35,NY=35,XX=2,YY=2.5,IM=1, COMM='Deposition example'; SUBS:PH=1E12,BO=1E13,AS=1E12,OR=111; BODE:XD=3 CS=1.E18; ANNE:TC=1000,TM=1800,TA=200 OX=0;} ASDE:XD=1 CS=1E20; ANNE:TC=1100,TM=1800,TA=100 OX=0;$
```

Buried layer and epitaxy

A substrate is doped by boron at 10^{16} cm⁻³, arsenic is implanted in the whole region at 300 KeV and 10^{15} ions/cm², and annealed at 1000 °C for 1 hour in an inert ambient. Epitaxy follows for

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10 minutes at 1200 °C resulting in a layer thickness of 2 microns which is doped by arsenic at 10^{15} cm⁻³. Then boron is implanted at 100 KeV and 10^{12} ions/cm² into the left side of the region and annealed at 1000 °C for 60 minutes. A nonuniform mesh is used.

```
MESH:NX=25,NY=38,XX=2,YY=3.5,IM=0,AX=1.E-5,AY=1,COMM='Buried layer example'; SUBS:PH=1E12,BO=1E16,AS=1E12,OR=111; ASIM:XM=10 EN=300. DZ=1E15; ANNE:TC=1000,TM=3600,TA=600 OX=0; EPIT:TH=2 PH=1.E12,BO=1.E12,AS=1.E15 TC=1200,TM=600,TA=150;} BOIM:XM=1. DZ=1.E12 EN=100; ANNE:TC=1000,TM=3600,TA=600 OX=0; $
```

Emitter region

To simulate emitter formation in the large fragment simulated in the previous example only its small upper region is considered. The substrate is doped by arsenic at 10^{15} cm⁻³ with boron implanted at 100 KeV and 10^{12} ions/cm² and arsenic implanted at 60 KeV and 10^{15} ions/cm² through the mask into the left half of the region. The wafer is then annealed for 1 hour at 1000 °C. The mesh is nonuniform in order to resolve a steep initial arsenic profile near the surface.

```
MESH:NX=15,NY=20,XX=1.,YY=1.1,IM=0 AX=1.E-5 AY=1., COMM='Emitter region'; SUBS:PH=1E12,BO=1E12,AS=1E15,OR=111; BOIM:XM=2 DZ=1.E12 EN=100; ASIM:XM=0.5 DZ=1.E15 EN=60; ANNE:TC=1000,TM=3600,TA=600 OX=0;$
```

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DEVICE FORMATION

Chapter 5 Device formation

5.1. Introduction

MergIC provides an interface between the process simulation tool SiDif and the device simulation tool SemSim. MergIC merges device fragments simulated by SiDif into a device domain to be used in the device simulation. The fragments may be placed arbitrarily in the device domain, symmetrized and replicated. The output file of MergIC serves as the numerical doping input file for SemSim.

MergIC allows one to significantly reduce the fragment size used in the process simulation and hence the CPU time. This also significantly simplifies mesh generation for the process simulation.

5.2. Running MergIC

To run **MergIC** from the **MicroTec** shell:

- Select a project corresponding to MergIC or add a new project by selecting MergIC method
 in the Method window. MergIC requires the main input file with the extension *.INP and one
 doping data file for every fragment used in the device structure. These fragment doping files
 must be previously generated by SiDif.
- Edit parameters by switching to "**Project Settings**" page of the in the main **MicroTec** menu.
- Click **Run** button.

To run **SemSim** outside the **MicroTec** shell the command line should look as follows:

mergic project>.inp

Refer to sections below for the description of the input file.

On the output **MergIC** generates a doping data file which is used in a device simulation by **SemSim**. If you want to plot the output doping file, click "**3D Output**" in the main **MicroTec** menu after running **MergIC**.

Note: Since the device simulation tool **SemSim** in the present version of **MicroTec** does not handle non-planar structures, a planarization of the doping profiles is made in **MergIC**. Therefore vertical doping profiles generated by **SiDif** are shifted vertically so as to align the Si/SiO_2 interface with the line y = 0. At the same time the impurity concentration values at y locations beyond the original domain generated by **SiDif** are filled with the value of the last point available, i.e. the bottom impurity concentration value in the **SiDif** output file.

5.3. MergIC input file

- Each directive starts a group of parameters separated by spaces or commas and ended by ';'.
- Each FRAG directive must be ended by "}". The last directive must be ended by \$.

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• All directives after \$ will be ignored.

MESH: Domain and mesh

Name	Default	Units	Description
NX			Number of nodes in X-direction (along the surface), it must be greater than 3.
NY			Number of nodes in Y-direction (into the depth of the domain). It must be greater than 3. The number of nodes affects accuracy and disk space required for the output file.
XX			Device size in X-direction (um).
YY			Device size in Y-direction (um).
COMM	'Comm'	none	Comment line.

FRAG: fragment description

Name	Default	Units	Description
X0	0	um	X-coordinate of the upper left corner of fragment in the device domain (um). It can exceed the overall length of the device if you want to invert the fragment over the vertical symmetry axis.
SY	0	none	Type of the fragment symmetrization. If SY=0 there is no fragment symmetrization. SY=1 means symmetrization over its right edge that is the fragment is extended symmetrically to the right, and SY=-1 means symmetrization over the left edge, or extension to the left.
DX	0	um	Length of the fragment extension, or a piece fitted between the symmetrical regions. It must be larger than 0. It is ignored if SY=0. This region is filled with the doping profile from the fragment borders which face each other.

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Name	Default	Units	Description
OV	1	none	Extension of the doping profile of the fragment to the whole device domain. It is needed to create the basic structure, for example, the initial doping, implantation to the whole device domain or buried layer. If OV=1, the doping values on the bottom edge of the fragment are continued to the bottom of the device domain, and then the profiles on the right and left edges of the fitted fragment are extended uniformly to the right and left borders of the device domain respectively. If OV=0, the fragment is placed over the region replacing the doping which was there before. No extension to the right, left or down is made in this case. OV=1 option is preferable for the first fragment.
IF			Name of the SiDif output file with the doping data for the fragment. It must be separated by ''.

5.4. Examples of MergIC input file

Examples of **MergIC** input files follow. The last three examples differ only in the way the fragments are placed.

Viewing a fragment

MESH: NX=50 NY=45 XX=5 YY=3, COMM='Fragment view'; FRAG:X0=0 DX=0 SY=0 OV=1 IF='MOS.OUD'\$

Symmetrical device using one fragment

MESH:NX=70 NY=40 XX=2.5 YY=1, COMM='NMOS Transistor'; FRAG:X0=1.6 DX=0.7 SY=-1 OV=1 IF='EXMOS.OUD'}\$

Vertical BJT with substrate collector

MESH:NX=150 NY=40 XX=5 YY=2.5, COMM='Vertical BJT'; FRAG:X0=4.5 DX=1 SY=0 OV=1 IF='BUR.OUD';} FRAG:X0=1 DX=1 SY=-1 OV=0 IF='EMIT.OUD';\$

Vertical BJT with a buried layer

MESH:NX=200 NY=40 XX=8 YY=3.5, COMM='Planar transistor';

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FRAG:X0=4. DX=1 SY=0 OV=1 IF='BUR.OUD';} FRAG:X0=1 DX=1 SY=-1 OV=0 IF='EMIT.OUD';\$

I²L Device

MESH:NX=200 NY=40 XX=10 YY=2.5, COMM='I2L device'; FRAG:X0=1 DX=1 SY=1 OV=1 IF='BUR.OUD';} FRAG:X0=10 DX=1 SY=-1 OV=0 IF='EMIT.OUD';\$

DEVICE SIMULATION

6.1. Introduction

A number of software tools are available for two-dimensional semiconductor device simulation. Conventionally they use Newton-like methods and this results in numerical instability and relatively high memory requirements.

Recently new methods for the linearization of the semiconductor equations were proposed [3,4,5] permitting the efficient solution of the nonlinear semiconductor equations. The methods use the "decoupled", or Gummel-like scheme [14], significantly reducing the memory requirements. Surprisingly, these methods appear to be more efficient than the Newton method in a number of instances and certainly are numerically more stable than the latter.

SemSim, as well as its predecessors **SiMOS** [1] and **BiSim** [2], is based on the Gummel-like decoupled technique and require only 4 Kbyte of memory for a 10,000 node mesh. A finite difference technique on a rectangular grid is employed. For discretization of the continuity equations the conventional Scharfetter-Gummel approximation [11] is used. Conjugate gradient methods with preconditioning [12,13] are used for solving the linear systems.

6.2. Basic System of Equations

The basic equations comprise of the Poisson equation (standard notation is used) and the continuity equations for electrons and holes

$$\nabla^2 \Psi = -\frac{q}{\varepsilon \varepsilon_0} (-n + p + N_D - N_A) , \qquad (6.1)$$

$$\frac{1}{q}\nabla J_n = (R - G) , \qquad (6.2)$$

$$-\frac{1}{q}\nabla J_p = (R - G) , \qquad (6.3)$$

where J_n , J_p are related to the carrier densities and the electrostatic potential

$$J_n = -qn\mu_n \nabla(\psi + \chi) + qD_n \nabla n , \qquad (6.4)$$

$$J_p = -qp\mu_p \nabla(\psi - \chi) - qD_p \nabla p . \qquad (6.5)$$

(6.6)

Bandgap narrowing

The additional term χ in the drift components of (4,5) is due to the band-gap narrowing effects and is treated accordingly to the Slotboom model [6]

$$\chi = -\frac{\Delta E_g}{2} = \chi_0 \left(ln \left(\frac{N}{N_c} \right) + \left(ln^2 \left(\frac{N}{N_c} \right) + L \right)^{\frac{1}{2}} \right) , \qquad (6.7)$$

where $N = N_D + N_A$.

Temperature dependence of the bandgap is as follows

$$E_g(T) = E_g(0) + \frac{E_{g\alpha}T^2}{T + E_{g\beta}} . ag{6.8}$$

Intrinsic carrier concentration is

$$n_{ie}(T) = \sqrt{N_C N_C} \exp\left(-\frac{E_g}{2kT}\right) \tag{6.9}$$

Effective density of states

$$N_C(T) = N_C(300) \left(\frac{T}{300}\right)^{3/2} \tag{6.10}$$

$$N_V(T) = N_V(300) \left(\frac{T}{300}\right)^{3/2} \tag{6.11}$$

SRH and Auger Recombination and Impact Ionization

The Shockley-Read-Hall recombination, Auger recombination and avalanche generation are taken into account

$$(R-G) = (R-G)_{SRH} + (R-G)_{Auger} - G_{av}$$
, (6.12)

$$(R-G)_{SRH} = \frac{np - n_{ie}^2}{(n+n_{ie})\tau_p + (p+n_{ie})\tau_n} , \qquad (6.13)$$

$$(R-G)_{Auger} = (np - n_{ie}^2)(C_n n + C_p p) , \qquad (6.14)$$

using concentration dependent lifetimes

$$\tau_n = \frac{\tau_{n0}}{\left(A_n + \left(B_n \left(\frac{N}{N_{n,ref}}\right) + C_n \left(\frac{N}{N_{n,ref}}\right)^{\alpha_n}\right)\right)},$$
(6.15)

and an analogous expression for holes.

Impact ionization is modeled using the Chynoweth model [7]

$$G_{av} = \alpha_n |J_n| + \alpha_p |J_p|, \qquad (6.16)$$

where

$$\alpha_n = a_n exp\left(\frac{-b_n|J_n|}{|(E \cdot J_n)|}\right) \text{ and } \alpha_p = a_p exp\left(\frac{-b_p|J_p|}{|(E \cdot J_p)|}\right). \tag{6.17}$$

Surface Recombination

Surface recombination takes place at the interfaces semiconductor/oxide or at the surface of non-ideal (for example polysilicon or Schottky) contacts. The recombination rate is described by the formula

$$(R-G)_{surf} = \frac{np - n_{ie}^2}{(n+n_{ie})/v_{sp} + (p+n_{ie})/v_{sn}} , \qquad (6.18)$$

where v_{sn} , v_{sp} are recombination velocities for electrons and holes.

Boundary Conditions

A few types of boundary conditions are available in **SemSim**. At ideal Ohmic contacts the following conditions are imposed (assuming infinite recombination rate for electrons and holes)

$$n_0 = \sqrt{N_N^2/4 + n_{ie}^2} + N_N/2, \qquad (6.19)$$

$$p_0 = \sqrt{N_N^2/4 + n_{ie}^2} - N_N/2, (6.20)$$

$$\Psi_0 = \frac{kT}{q} \ln \left(\frac{n_0}{n_{io}} \right) + V_k \,, \tag{6.21}$$

where $N_N = N_D - N_A$ is the net doping concentration and V_k is the k-th contact voltage.

On the surface of Schottky contacts (**BiSim** only) carrier concentrations are defined by the following relations

$$J_{n, y} = q v_{sn} (n - n_{eq}) , (6.22)$$

$$J_{p,v} = -qv_{sp}(p - p_{eq}) , (6.23)$$

$$\Psi_0 = -\Phi_R + V_k, \tag{6.24}$$

where Φ_B is the difference of the intrinsic semiconductor and metal workfunctions, ν denotes current density component normal to the interface, and equilibrium concentrations n_{eq} , p_{eq} are

$$n_{eq} = n_{ie} \exp\left(\frac{q\Psi_0}{kT}\right),\tag{6.25}$$

$$p_{eq} = n_{ie} \exp\left(-\frac{q\psi_0}{kT}\right). \tag{6.26}$$

On insulating segments of the boundary for current densities we have

$$J_{n, \nu} = q(R - G)_{surf}, \qquad (6.27)$$

$$J_{p, v} = -q(R - G)_{surf}. (6.28)$$

For normal components of electric field according to the Gauss theorem we have at the interface

$$\varepsilon_1 E_{1,y} = \varepsilon_2 E_{2,y} + Q_{ss} \tag{6.29}$$

where ε_1 , ε_2 are dielectric permittivities of the respective materials and Q_{ss} is a fixed surface charge density. For open segments of the boundary $E_{2, v}$ equals zero. For boundary segments underneath gate contacts the electric field is approximated by the formula

$$E_{2, v} = -\frac{(V_{G, eff} - \psi_s)}{h_d} \tag{6.30}$$

where $V_{G, eff} = V_{G, appl} - \Phi_B$, h_d is the oxide thickness, and ψ_s is the local potential value at the interface.

Mobility Models

Several options for concentration and field dependent mobility models are available. For bipolar devices the concentration and field dependent mobility is taken in a form similar to [8]

$$\mu_{S,n}(N, E_t) = G_{surf,n} \left(\mu_n^{min} + \frac{\mu_n^{max} \left(\frac{T}{300} \right)^{V_n} - \mu_n^{min}}{1 + \left(\frac{T}{300} \right)^{\xi_n} \left(\frac{N}{N_{ref,n}} \right)^{\alpha_n}} \right) \left(1 + \left| \frac{E_t}{E_{cn,\mu}} \right| \right)^{-\frac{1}{2}} , \qquad (6.31)$$

$$\mu_n(N, E_t, E_l) = \mu_{S, n}(N, E_t) \left(1 + \left(\frac{\mu_{S, n} E_l}{\nu_{sat, n}} \right)^{\beta_n} \right)^{-\frac{1}{\beta_n}},$$
(6.32)

And analogous expression for holes.

For MOS devices either the Yamaguchi expression [9] or the recent expression by Lombardi et al [10] may be used. In the first case [9]

$$\mu_n(N, E_l, E_t) = \mu_1(N, E_t) \left(1 + \frac{\left(\frac{\mu_1 E_l}{v_c}\right)^2}{G + \left(\frac{\mu_1 E_l}{v_c}\right)} + \left(\frac{\mu_1 E_l}{v_s}\right)^2 \right)^{-\frac{1}{2}}, \tag{6.33}$$

$$\mu_1(N, E_t) = \mu_0 \left(1 + \frac{N}{N_r + \frac{N}{S}} \right)^{-1} \left(1 + \alpha |E_t| \right)^{-\frac{1}{2}}, \tag{6.34}$$

where E_l and E_t are corresponding longitudinal and transverse components of the electric field with respect to the current direction. In the second case [10] the mobility includes three terms

$$\frac{1}{\mu} = \frac{1}{\mu_{ac}} + \frac{1}{\mu_b} + \frac{1}{\mu_{sr}}.$$
 (6.35)

where μ_{ac} is the carrier mobility limited by the surface acoustic phonon scattering, μ_b is the carrier mobility in the bulk silicon, and μ_{sr} is the carrier mobility limited by the surface roughness scattering. These terms are described by the following formulae

$$\mu_{ac}(E_t, T) = \begin{pmatrix} B \frac{T}{E_t} + \frac{C}{\frac{1}{2}} \\ E_t^{\frac{3}{2}} \end{pmatrix};$$
 (6.36)

$$\mu_b(N, T) = \mu_0 + \frac{\mu_{max(T)} - \mu_0}{1 + \left(\frac{N}{C_r}\right)^{\alpha}} - \frac{\mu_1}{1 + \left(\frac{C_s}{N}\right)^{\beta}} ; \qquad (6.37)$$

where
$$\mu_{max(T)} = \mu_{max} \left(\frac{T}{300}\right)^{-\gamma}$$
, and $\mu_{sr} = \frac{\delta}{E_t^2}$.

The basic parameters in the above expressions are user defined.

6.3. Numerical technique

A finite difference technique on a rectangular grid, is used together with a decoupled method of iterating over the non-linearity (the so called Gummel iteration). For discretization of the continuity equations we use the conventional Scharfetter-Gummel approximation [11]. Conjugate gradient methods with preconditioning [12,13] are available for solving the linear systems.

6.4. References

- [1] M. S. Obrecht, "SIMOS two-dimensional steady-state simulator for MOS-devices". Solid-State Electronics, Software Survey Section, vol. 32, No. 6, 1989.
- [2] M. S. Obrecht and J. M. G. Teven, "BISIM a program for steady-state two-dimensional modeling of various bipolar devices". Solid-State Electronics, Software Survey Section, vol. 34, No.7, 1991.
- [3] M. S. Obrecht, "A new stable method for linearization of discretized basic semiconductor equations", Solid State Electronics, vol.36, No.4, pp. 643-648, 1993.
- [4] M. S. Obrecht and M. I. Elmasry, "Speeding-up of convergence of Gummel iterations for

- transient simulation", Proceedings of the Ninth International Conference on the Numerical Analysis of Semiconductor Devices and Integrated Circuits, Copper Mountains, CO, April 6-8, 1993, Front Range Press, pp.20-21
- [5] M. S. Obrecht and M. I. Elmasry, "Speeding-up of convergence of Gummel iterations for transient simulation", COMPEL, v. 12, pp. 311-317.
- [6] J. V. Slotboom and H. C. De Graaf, "Measurements of bandgap narrowing in silicon bipolar transistor", Solid-State Electronics, vol. 19, pp. 857-862, 1976.
- [7] A. G. Chynoweth, "Ionization rates for electrons and holes in silicon", Phys.Rev., vol. 109, pp.1537-1540, 1958.
- [8] D. M. Caughey and R. E. Thomas, "Carrier mobilities in silicon semi-empirically related to temperature, doping and injection level", Proc.IEEE, vol. 55, pp. 2192-2193, 1967.
- [9] K. Yamaguchi, "A mobility model for carriers in the MOS inversion layer", IEEE Trans. Electron Devices, vol. 30, pp.658-663, 1983.
- [10] C. Lombardi, S. Manzini, A. Saporito and M. Vanzi, "A physically based mobility model for numerical simulation of nonplanar devices," IEEE Trans. Computer Aided Design, vol. 7, pp. 1164-1170, November 1988.
- [11] D. L. Scharfetter, H. K. Gummel,: "Numerical simulation of Read diode oscillator", IEEE Trans. Electron Devices, vol. 16, pp.64-70, 1969.
- [12] M. S. Obrecht "A modification of ICCG method for solving discretized continuity equations for semiconductor device at any voltages," Submitted to Solid State Electronics.
- [13] H. A. Van Der Vorst, "Bi-CGSTAB: a fast and smoothly converging variant of Bi-CG for the solution of nonsymmetric linear systems," SIAM Journ. Sci. Stat. Comput., vol. 13, pp. 631-644, March 1992.
- [14] H. K. Gummel, "A self-consistent iterative scheme for one-dimensional steady-state transistor calculations", IEEE Trans. Electron Devices, vol.11, pp. 455-465, 1964.
- [15] A. De Mari, "An accurate numerical steady-state one-dimensional solution of the p-n junction," Solid-St. Electronics, vol. 11, p. 33-58, 1968.
- [16] M. S. Mock, "A time-dependent numerical model of the insulated-gate field-effect transistor", Solid State Electronics, vol.24, pp.959-966, 1981.

6.5. Running SemSim

To run **SemSim** from the **MicroTec** shell:

- Select a project corresponding to SemSim or add a new project by selecting SemSim method in the Method window
- Edit parameters by switching to "Project Settings" page of the in the main MicroTec menu
- Click Run button.

To run **SemSim** outside the **MicroTec** the command line should look as follows

semsim project>.inp

File "inst.pas" must be present in the directory where **MicroTec** is installed.

There are two output files generated by **SemSim**:

- 1. A file with two-dimensional distributions. It has the extension *.3D.
- 2. A file with I-V data. It has the extension *.2D.

These two files may be displayed by **MicroTec** graphics tools. Click on the **2D** or **3D** button in the **MicroTec** main menu to plot the results.

Refer to sections below for the description of the input file.

6.6. SemSim input file

SemSim main input file contains directives, subdirectives and parameters. Each directive contains subdirectives or parameters, starts with the directive key followed by ':' and should be ended by '}'. Each subdirective contains parameters, separated by spaces or commas. They start with the subdirective key followed by ':' and ended by ';'. Input is closed by '\$', all directives after '\$' are ignored.

Directive/subdirective tree looks as follows.

•#BAS: Basic directives

MESH: Mesh and domain parametersSOLV: Numerical solution parameters

•MODE: Physical models

• #DOP: Analytical doping data

•DOPA: Doping well

•DOPN: Numerical doping data from file

•#ELE: Electrodes

•OHMI: Ohmic electrode •GATE: Gate electrode •SCHO: Schottky electrode

•#IVD: IV-data or a set of IV-curves

•IVDA: IV-curve

•#MAT: Material Properties

BAND: Temperature and bandgapPERM: Dielectric permittivity

•WORK: Workfunction

•#MOB: Mobility models

CONM: Constant mobilityYAMA: Yamaguchi mobilityLOMB: Lombardi mobilityBIPO: Bipolar mobility

•#REC: Recombination parameters

•SRH: Shockley-Read-Hall recombination parameters

•AUGE: Auger recombination parameters

•SURF: Surface recombination •RADI: Radiative recombination

•#IMP: Impact ionization

•IONE: Impact ionization exponents•IONP: Impact ionization coefficients

•#PHO: Photogeneration

•PHOT: Photogeneration well

#BAS: Basic directives

This directive includes the following three unique directives: **MESH**, **SOLV** and **MODE**.

MESH: Domain and mesh parameters

Name	Default	Units	Description
NX	30	none	Number of mesh nodes in X direction, along the wafer surface. It must be greater than 3. A greater number of mesh nodes gives a higher computational accuracy at the expense of a larger CPU time.
NY	30	none	Number of mesh nodes in Y direction, into the depth of the wafer. It must be greater than 3.
XX	1	um	Domain size in X-direction, microns.
YY	1	um	Domain size in Y-direction.
ZZ	1	um	Domain size in Z-direction, in other words device width.
HY0	0.01	um	Y-direction first step size, used only if IMESH is equal to 0.

Name	Default	Units	Description
MESH	2	none	If MESH=0, the mesh size is constant in X direction and exponentially growing in Y direction. If MESH=1, mesh data are to be read from file. If MESH=2, automatic remeshing is performed in both X and Y directions. If MESH=3 or 4 remeshing is done only for X or Y directions respectively.

SOLV: Computation control

Name	Default	Units	Description	
COMM	'Comm'	none	Comment line to be written in the output file	
BATC	1	none	If BATC=1, simulate without interactive plotting after every IV-point, if BATC=0, otherwise.	
GUMM	100	none	Number of Gummel iterations for closure. Iteration stops when either the Gummel residual or the maximum number of Gummel iteration has been reached.	
GRES	0.01	kT/q	Gummel residual criterion for closure. Iteration stops when either the Gummel residual or the maximum number of Gummel iteration has been reached.	

MODE: Model options

Name	Default	Units	Description	
ELHL	0	none	Solve continuity equations for both carriers if ELHL=0. Solve for electrons or holes only if ELHL is equal 1 or 2 respectively.	
HVDO	1	none	Use Slotboom heavy doping bandgap narrowing model if HVDO=1 and otherwise if HVDO=0.	
IMPI	0	none	Use Chinoweth impact ionization model if IMPI=1 and otherwise if IMPI=0.	

#DOP: Analytical doping data

This directive may include any number of **DOPA**: subdirectives. The analytical doping profiles are described by a superposition of wells. For each well is defined by one **DOPA**: subdirective according to the following formula

$$N_{well} = N_0 \exp\left(-\left(\frac{f(x_l - x)}{L_x}\right)^2 - \left(\frac{f(x - x_r)}{L_x}\right)^2 - \left(\frac{f(y - y_b)}{L_y}\right)^2 - \left(\frac{f(y_t - y)}{L_y}\right)^2\right)$$

$$f(x) = \frac{|x| + x}{2}$$

The concentration in every well is a constant equal to N_0 in the rectangle X_{left} , Y_{top} , X_{right} , Y_{bottom} and decreases as a Gaussian beyond the rectangle. N_0 is the maximum concentration in the well, it is positive for donors and negative for acceptors.

DOPA: Doping well

Name	Default	Units	Description	
COMM	Comm	none	Doping well name	
DOP	1.1018	cm ⁻³	Maximum concentration in the doping well.	
XLFT	0	um	Left edge of the doping well.	
XRGT	1	um	Right edge of the doping well.	
YTOP	0	um	Top of the doping well.	
YBOT	1	um	Bottom of the doping well.	
ALX	0.05	um	Characteristic length in X direction.	
ALY	0.07	um	Characteristic length in Y direction.	

DOPN: Numerical doping data

The only parameter in this directive is the doping data file name. In this case the doping data file should contain doping data generated by **SiDif** or post-processed by **MergIC** which, in turn, uses output files generated by the process simulator **SiDif**.

Name	Default	Units	Description
FILE		none	Name of the file where data, previously evaluated using SiDif or MergIC are stored.

#ELE: Electrode directive

OHMI: Ohmic electrode

Name	Default	Units	Description	
NAME	'ohmic'	none	Electrode name. The first letter will be used for current and voltage subscripts.	
NUM	1	none	Electrode number. Important when setting initial voltages and voltage step in IV-data.	
LOC	1	none	Location of the electrode, 1 is on the top and 2 is on the bottom of the domain.	
XLT	0	um	Left electrode edge coordinate.	
XRT	1	um	Right electrode edge coordinate.	

GATE: Gate electrode

Name	Default	Units	Description	
NAME	'gate'	none	Electrode name. The first letter will be used for current and voltage subscripts.	
NUM	1	none	Electrode number. Important when setting initial voltages and voltage step in IV-data.	
LOC	1	none	Location of the electrode, 1 is on the top and 2 is on the bottom of the domain.	
XLT	0	um	Left electrode edge coordinate.	
XRT	1	um	Right electrode edge coordinate.	
TOX	0.02	um	Gate oxide thickness.	
XQS	0.01	um	Location of the Gaussian Qss under the gate.	
AQS	0.01	um	Exponent of the Gaussian Qss under the gate.	
QSH	0	cm ⁻²	Homogeneous component of the Qss under the gate.	
QSG	0	cm ⁻²	Gaussian component of the Qss under the gate.	
VSN	1·10 ⁻¹⁵	cm/s	Electron recombination velocity under the gate.	
VSP	1·10 ⁻¹⁵	cm/s	Hole recombination velocity under the gate.	
FIM	4.25	eV	Work function of the gate metal.	

Parameters x_{QS} , A_{QS} , Q_{SH} , Q_{SG} define slow surface states, or fixed surface charge, at the Si/SiO2 interface as follows

$$Q_{SS} = Q_{SH} + Q_{SG} \exp\left(-\left(\frac{(x - x_{QS})}{A_{QS}}\right)^2\right) .$$

SCHO: Schottky electrode

Name	Default	Units	Description	
NAME	'schottky'	none	Electrode name. The first letter will be used for current and voltage subscripts.	
NUM	1	none	Electrode number. Important when setting initial voltages and voltage step in IV-data.	
LOC	1	none	Location of the electrode, 1 is on the top and 2 is on the bottom of the domain.	
XLT	0	um	Left electrode edge coordinate.	
XRT	1	um	Right electrode edge coordinate.	
VSN	1.105	cm/s	Electron recombination velocity at the interface.	
VSP	1.105	cm/s	Hole recombination velocity at the interface.	
FIB	0	eV	Potential barrier: the difference between the Fermi potential of the contact material and that of the intrinsic semiconductor.	

#IVD: IV-data directive

This directive may include any number of **IVDA**: subdirectives. Each **IVDA**: subdirective defines one IV-curve for which one the contact voltages is ramped.

IVDA: IV-Curve

Name	Default	Units	Description	
TEXT		none	Text to be output to the IV-data file.	
NUMC	1	none	Number of the contact to sweep the voltage.	
NPNT	1	none	Number of IV-points to be evaluated.	

Name	Default	Units	Description	
VSTE	0.1	V	Voltage step size.	
V1	0	V	Initial voltage for contact #1	
V2	0	V	Initial voltage for contact #2	
V3-V20	0	V	Same as above, just a repetition. Initial voltage for a contact #3 - #20. Maximum contact number is equal to 20.	

#MAT: Material properties

This directive contains three unique subdirectives: **BAND**, **PERM** and **WORK**.

BAND: Temperature and bandgap parameters

$$\chi = -\frac{\Delta E_g}{2} = V_{0,BGN} \left(ln \left(\frac{N}{N_{0,BGN}} \right) + \left(ln^2 \left(\frac{N}{N_{0,BGN}} \right) + C_{BGN} \right)^{\frac{1}{2}} \right) ,$$

$$E_g(T) = E_g(300) + E_{g\alpha} \left(\frac{300^2}{300 + E_{g\beta}} - \frac{T^2}{T + E_{g\beta}} \right) .$$

$$N_C(T) = N_C(300) \left(\frac{T}{300} \right)^{3/2} , \quad N_V(T) = N_V(300) \left(\frac{T}{300} \right)^{3/2} .$$

Symbol	Name	Default	Units	Description
T	TEMP	300	K	Temperature
$E_g(300)$	EG30	1.08	eV	Bandgap width at 300 K
$E_{g\alpha}$	EGAL	4.73·10 ⁻⁴	eV	Value of Alpha in the formula for the bandgap width
$E_{g\beta}$	EGBE	6.36·10 ²	° K	Temperature correction term in the formula for the bandgap width
<i>N_C</i> (300)	ENC3	2.8·10 ¹⁹	cm ⁻³	The semiconductor conduction band density of states

Symbol	Name	Default	Units	Description
N _V (300)	ENV3	1.04·10 ¹⁹	cm ⁻³	The semiconductor valence band density of states
$V_{0,BGN}$	V0BG	0.009	eV	The voltage parameter in the bandgap narrowing model
$N_{0,BGN}$	CONB	1.0·10 ¹⁷	cm ⁻³	The concentration parameter in the bandgap narrowing model
C_{BGN}	CNSB	0.5	none	The constant parameter in the bandgap narrowing model

PERM: Dielectric permittivity

Name	Default	Units	Description
EPSD	3.9	none	The relative dielectric permittivity of the oxide
EPSS	11.8	none	The relative dielectric permittivity of the semiconductor

WORK: Semiconductor work function

Name	Default	Units	Description
FIS	4.17	eV	Semiconductor electron affinity

#MOB: Mobility models

This directive contains four unique subdirectives: CONM, YAMA, LOMB and BIPO.

CONM: Constant mobility model

Symbol	Name	Default	Units	Description
$\mu_{n, 0}$	UMN0	1000	cm ² /V·s	Constant mobility for electrons
$\mu_{p,0}$	UMP0	500	cm ² /V·s	Constant mobility for holes

YAMA: Yamaguchi mobility model

$$\mu_n(N, E_l, E_t) = \mu_1(N, E_t) \left(1 + \frac{\left(\frac{\mu_1 E_l}{v_c}\right)^2}{G + \left(\frac{\mu_1 E_l}{v_c}\right)} + \left(\frac{\mu_1 E_l}{v_s}\right)^2 \right)^{-\frac{1}{2}},$$

$$\mu_1(N, E_t) = \mu_0 \left(1 + \frac{N}{N_r + \frac{N}{S}}\right)^{-1} \left(1 + \alpha |E_t|\right)^{-\frac{1}{2}},$$

Symbol	Name	Default	Units	Description
μ_{n0}	UMN0	1.4·10 ³	cm ² /Vs	Maximum electron mobility
S_n	SN	350.0	none	Doping concentration factor for electrons
N_{rn}	RSN	3.0·10 ¹⁶	cm ⁻³	Reference doping concentration for electrons
α_n	ALN	1.54·10 ⁻⁵	cm/V	Perpendicular electric field factor for electrons
V_{sn}	VSN	1.036·10 ⁷	cm/s	Saturation velocity for electrons
G_n	GN	8.8	none	Parallel electric filed factor for electrons
v_{cn}	VCN	4.9·10 ⁶	cm/s	Phonon velocity fitting parameter
μ_{p0}	UMP0	480.0	cm ² /V·s	Maximum hole mobility
S_p	SP	81.0	none	Doping concentration factor for electrons
N_{rp}	RSP	4.0·10 ¹⁶	cm ⁻³	Reference doping concentration for holes
α_p	ALP	5.35·10 ⁻⁵	cm/V	Perpendicular electric field factor for holes
v_{sp}	VSP	1.2·10 ⁷	cm/s	Saturation velocity for holes

Symbol	Name	Default	Units	Description
G_p	GP	1.6	none	Parallel electric filed factor for holes
v_{cp}	VCP	2.928·10 ⁶	cm/s	Phonon velocity fitting parameter

LOMB: Lombardi surface mobility model

$$\frac{1}{\mu} = \frac{1}{\mu_{ac}} + \frac{1}{\mu_b} + \frac{1}{\mu_{sr}}, \qquad \mu_{ac}(E_t, T) = \left(B\frac{T}{E_t} + \frac{C_0 N^{\theta}}{\frac{1}{E_t^3}}\right), \mu_{sr} = \frac{\delta}{E_t^2}$$

$$\mu_b(N, T) = \mu_0 + \frac{\mu_{max(T)} - \mu_0}{1 + \left(\frac{N}{C_r}\right)^{\alpha}} - \frac{\mu_1}{1 + \left(\frac{C_s}{N}\right)^{\beta}} ; \quad \mu_{max}(T) = \mu_{max} \left(\frac{T}{300}\right)^{-\gamma} .$$

$$\mu_{n}(N, E_{t}, E_{l}, T) = \mu_{n}(N, E_{t}, T) \left(1 + \left(\frac{\mu_{S, n} E_{l}}{v_{sat, n}}\right)^{\beta_{sat, n}}\right)^{\frac{1}{\beta_{sat, n}}},$$

Symbol	Name	Default	Units	Description
В	BN	4.75·10 ⁷	cm/s	Fitting parameter for perpendicular electric filed
C_o	C0N	1.74·10 ⁵		Fitting parameter for perpendicular electric filed and doping concentration
θ	CPON	0.125	none	Exponent of the doping concentration parameter
μ_0	U0N	52.2	cm ² /V·s	Minimum hole mobility
μ_{max}	UMAN	1.42·10 ³	cm ² /V·s	Maximum hole mobility
μ_1	ULN	43.4	cm ² /V·s	Concentration correction term
C_r	CRN	9.68·10 ¹⁶	cm ⁻³	Critical doping concentration
C_s	CSN	3.43·10 ²⁰	cm ⁻³	Critical doping concentration in the correction term

Symbol	Name	Default	Units	Description
P_c	PCN	0.0	cm/s	Concentration correction of the minimum mobility
α	ALPN	0.68	none	Exponent in the concentration factor
β	BETN	2.0	none	Exponent in the concentration correction factor
γ	GAMN	2.5	none	Temperature factor exponent
δ	DELN	5.82·10 ¹⁴	V/s	Acoustic term parameter
$\beta_{sat, n}$	BESN	2.0	none	Exponent in the saturation velocity
v _{sat, n}	VSAN	1.07·10 ⁷	cm/s	Saturation velocity

Analogous parameters for holes (note that expression for $\mu_{\it b}$ in this case is different)

$$\mu_b(N, T) = \mu_0 \exp(-P_c/N) + \frac{\mu_{max(T)}}{1 + \left(\frac{N}{C_r}\right)^{\alpha}} - \frac{\mu_1}{1 + \left(\frac{C_s}{N}\right)^{\beta}}$$

Symbol	Name	Default	Units	Description
В	BP	9.93·10 ⁷	cm/s	Fitting parameter for perpendicular electric filed
C_o	СОР	8.84·10 ⁵		Fitting parameter for perpendicular electric filed and doping concentration
θ	СРОР	3.17·10 ⁻²	none	Exponent of the doping concentration parameter
μ_0	U0P	44.9	cm ² /V·s	Minimum electron mobility
μ_{max}	UMAP	470	cm ² /V·s	Maximum electron mobility
μ_1	ULP	29	cm ² /V·s	Concentration correction term
C_r	CRP	2.23·10 ¹⁷	cm ⁻³	Critical doping concentration
C_s	CSP	6.10.10 ²⁰	cm ⁻³	Critical doping concentration in the correction term

Symbol	Name	Default	Units	Description
P_c	PCP	9.23·10 ¹⁶	cm/s	Concentration correction of the minimum mobility
α	ALPP	0.719	none	Exponent in the concentration factor
β	BETP	2.0	none	Exponent in the concentration correction factor
γ	GAMP	2.2	none	Temperature factor exponent
δ	DELP	2.05·10 ¹⁴	V/s	Acoustic term parameter
$\beta_{sat, p}$	BESP	1.0	none	Exponent in the saturation velocity
v _{sat, p}	VSAP	1.07·10 ⁷	cm/s	Saturation velocity

BIPO: Bipolar mobility model

$$\mu_{S, n}(N, E_t) = G_{surf, n} \left(\mu_n^{min} + \frac{\mu_n^{max} \left(\frac{T}{300} \right)^{V_n} - \mu_n^{min}}{1 + \left(\frac{T}{300} \right)^{\xi_n} \left(\frac{N}{N_{ref, n}} \right)^{\alpha_n}} \right) \left(1 + \left| \frac{E_t}{E_{cn, \mu}} \right| \right)^{-\frac{1}{2}} ,$$

$$\mu_n(N, E_t, E_l) = \mu_{S, n}(N, E_t) \left(1 + \left(\frac{\mu_{S, n} E_l}{v_{sat, n}}\right)^{\beta_n}\right)^{-\frac{1}{\beta_n}},$$

Symbol	Name	Default	Units	Description
$\mu_{n, min}$	UMNM	55.2	cm ² /V·s	Minimum electron mobility
$\mu_{n, max}$	UMNX	1430	cm ² /V·s	Maximum electron mobility
$N_{ref, n}$	CRFN	1.07·10 ¹⁷	cm ⁻³	Reference impurity concentration for electrons
E_{cmn}	ECNM	6.49·10 ⁴	V/cm	Critical electric field in the perpendicular electric field mobility for electrons
v _{sat, n}	VSTN	1.07·10 ⁷	cm/s	Electron saturation velocity

Symbol	Name	Default	Units	Description
V_n	UNN	-2.3	none	Exponent of normalized temperature in the numerator for electrons
ξ_n	XIN	-3.8	none	Exponent of normalized temperature in the denominator for electrons
α_n	ALPN	0.733	none	Exponent of impurity concentration for electrons
$G_{surf, n}$	GSRN	1.0	none	Low-field reduction factor for electron mobility
β_n	BETN	2.0	none	Exponent used in the field-dependent electron mobility for parallel electric field
$\mu_{p, min}$	UMPM	49.7	cm ² /V·s	Minimum hole mobility
$\mu_{p, max}$	UMPX	479	cm ² /V·s	Maximum hole mobility
$N_{ref, p}$	CRFP	1.6·10 ¹⁷	cm ⁻³	Reference impurity concentration for holes
E_{cmp}	ECPM	1.87·10 ⁴	V/cm	Critical electric field in the perpendicular electric field mobility for holes
v _{sat, p}	VSTP	1.06·10 ⁷	cm/s	Hole saturation velocity
ν_p	UNP	-2.2	none	Exponent of normalized temperature in the numerator for holes
ξ_p	XIP	-3.7	none	Exponent of normalized temperature in the denominator for holes
α_p	ALPP	0.7	none	Exponent of impurity concentration for holes
$G_{surf, p}$	GSRP	1.0	none	Low-field reduction factor for hole mobility
β_p	ВЕТР	1.0	none	Exponent used in the field-dependent hole mobility for parallel electric field

#REC: Recombination parameters

This directive contains four unique subdirectives: SRH, AUGE, SURF and RADI.

SRH: Shockley-Read-Hall recombination parameters

$$(R - G)_{SRH} = \frac{np - n_{ie}^2}{(n + n_{ie} \exp(E_{tr}/kT))\tau_p + (p + n_{ie} \exp(-E_{tr}/kT))\tau_n} ,$$

$$\tau_n = \frac{\tau_{n0}}{\left(A_{SRH, n} + \left(B_{SRH, n}\left(\frac{N}{N_{SRH, n}}\right) + C_{SRH, n}\left(\frac{N}{N_{SRH, n}}\right)^{\alpha_{SRH, n}}\right)\right)} ,$$

$$\tau_p = \frac{\tau_{p0}}{\left(A_{SRH, p} + \left(B_{SRH, p}\left(\frac{N}{N_{SRH, p}}\right) + C_{SRH, p}\left(\frac{N}{N_{SRH, p}}\right)^{\alpha_{SRH, p}}\right)\right)} ,$$

Symbol	Name	Default	Units	Description
E_{tr}	ETRA	0.0	eV	Energy level of SRH trap relatively to the intrinsic Fermi level
τ_{n0}	TAUN	1.0.10-7	s	Life time for electrons
$N_{SRH, n}$	NSRN	5.0·10 ¹⁶	cm ⁻³	Concentration parameter
$A_{SRH, n}$	ANSR	1.0	none	parameter
$B_{SRH, n}$	BNSR	1.0	none	parameter
$C_{SRH, n}$	CNSR	0.0	none	parameter
$\alpha_{SRH, n}$	EN	2.0	none	parameter
τ_{p0}	TAUP	1.0·10 ⁻⁷	S	Life time for holes
$N_{SRH, p}$	NSRP	5.0·10 ¹⁶	cm ⁻³	Concentration parameter
$A_{SRH, p}$	APSR	1.0	none	parameter
$B_{SRH, p}$	BPSR	1.0	none	parameter
$C_{SRH, p}$	CPSR	0.0	none	parameter
$\alpha_{SRH, p}$	EP	2.0	none	parameter

AUGE: Auger recombination parameters

$$(R-G)_{Auger} = (np - n_{ie}^2)(C_{Aug,n}n + C_{Aug,p}p)$$
,

Symbol	Name	Default	Units	Description
$C_{Aug, n}$	AUGN	2.8·10 ⁻³¹	cm ⁶ /s	Auger recombination coefficient
$C_{Aug, p}$	AUGP	9.9·10 ⁻³²	cm ⁶ /s	Auger recombination coefficient

SURF: Surface recombination parameters

$$(R-G)_{surf} = \frac{np - n_{ie}^2}{(n + n_{ie})/v_{sp} + (p + n_{ie})/v_{sn}} ,$$

Symbol	Name	Default	Units	Description
v _{sn}	VSRN	1·10 ⁻¹⁰	cm/s	Surface recombination velocity for electrons
v_{sp}	VSRP	1·10 ⁻¹⁰	cm/s	Surface recombination velocity for electrons

RADI: Radiative recombination parameters

$$(R-G)_{rad} = B(np-n_{ie}^2) ,$$

Symbol	Name	Default	Units	Description
В	RATE	1·10 ⁻¹⁴	cm ⁻³ /s	Radiative recombination coefficient

#IMP: Impact Ionization

This directive contains two unique subdirectives: **IONE** and **IONP**.

IONE: Impact ionization exponent

$$G_{av} = \alpha_n |J_n| + \alpha_p |J_p|, \quad \alpha_n = a_n exp\left(\frac{-b_n |J_n|}{|(E \cdot J_n)|}\right), \quad \alpha_p = a_p exp\left(\frac{-b_p |J_p|}{|(E \cdot J_p)|}\right).$$

For four ranges of electric field 0-E $_0$, E $_0$ -E $_1$, E $_1$ -E $_2$, E $_2$ - infinity, piecewise coefficients a_n, a_p, b_n, b_p are defined below

Symbol	Name	Default	Units	Description
E ₀	EN0	0.0	V/cm	Electric field range 0-E ₀ for electrons
E ₁	EN1	4.0.105	V/cm	Electric field range E ₀ -E ₁ for electrons
E ₂	EN2	6.0.10 ⁵	V/cm	Electric field range E ₁ -E ₂ for electrons
b^{o}_{n}	BN0	0.0	V/cm	Field exponent for electrons in 0 - E ₀
b^{1}_{n}	BN1	1.4·10 ⁶	V/cm	Field exponent for electrons in E_0 - E_1
b_n^2	BN2	1.4·10 ⁶	V/cm	Field exponent for electrons in E_1 - E_2
b^3_n	BN3	1.4·10 ⁶	V/cm	Field exponent for electrons in E ₂ -
E ₀	EP0	0.0	V/cm	Electric field range for holes
E ₁	EP1	6.07·10 ⁵	V/cm	Electric field range for holes
E ₂	EP2	6.07·10 ⁵	V/cm	Electric field range for holes
b^{o}_{p}	BP0	0.0	V/cm	Field exponent for holes in 0 - E ₀
b^1_{p}	BP1	2.09·10 ⁶	V/cm	Field exponent for holes in E_0 - E_1
b^2_{p}	BP2	1.4·10 ⁶	V/cm	Field exponent for holes in E ₁ - E ₂
b^3_{p}	BP3	1.4·10 ⁶	V/cm	Field exponent for holes in E ₂ -
a^0_n	AN0	0.0	1/cm	Ioniz.coef.for elect. in range 0 - E ₀

IONP: Impact ionization coefficient

Symbol	Name	Default	Units	Description
a_n^0	AN0	0.0	1/cm	Ioniz.coef.for elect. in range 0 - E ₀
a_n^1	AN1	7.0·10 ⁵	1/cm	Ioniz.coef.for elect. in range E_0 - E_1
a_n^2	AN2	7.0·10 ⁵	1/cm	Ioniz.coef.for elect. in range E ₁ - E ₂
a_n^3	AN3	7.0·10 ⁵	1/cm	Ioniz.coef.for elect. in range E ₂ -
a^0_{p}	AP0	0.0	1/cm	Ioniz.coef.for holes in range 0 - E ₀
a^{1}_{p}	AP1	1.3·10 ⁶	1/cm	Ioniz.coef.for holes in range E_0 - E_1
a_{p}^{2}	AP2	4.4·10 ⁵	1/cm	Ioniz.coef.for holes in range E ₁ - E ₂
a^3_p	AP3	4.4·10 ⁵	1/cm	Ioniz.coef.for holes in range E ₂ - infinity

#PHO: Photogeneration

This directive may include any number of **PHOT** subdirectives. The photogeneration distribution is described by a superposition of photogeneration wells. Each well is defined by one **PHOT** subdirective similar to the analytical doping profile using subdirective **DOPA**.

PHOT: Photogeneration well

Name	Default	Units	Description
RATE	1.10 ²⁰	cm ⁻³ /s	Maximum photogeneration rate in the well.
XLFT	0	um	Left edge of the doping well.
XRGT	1	um	Right edge of the doping well.
YTOP	0	um	Top of the doping well.
YBOT	1	um	Bottom of the doping well.
ALX	0.001	um	Characteristic length in X direction.
ALY	0.001	um	Characteristic length in Y direction.