MicroTec

Software Package for Two-Dimensional Process and Device Simulation

Version 4.0 for Windows

User's Manual

Siborg Systems Inc

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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 sized meshes.

Increasing performance and widespread 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 completeness and ease of use. 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 teach 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 its apparent simplicity, **MicroTec** covers all the basic needs of 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 the 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-4.0 is a true 32-bit Windows application and can be run on any PC-386 or higher. **MicroTec**-4.0 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 to 3,500 nodes. **MicroTec**-4.0 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 memory requirements, 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 will need about 4 Megabytes of disk space to install **MicroTec**-4.0.

1. Create directory C:\MT305 on a hard disk

2. Copy all MicroTec files from the floppy into this directory

3. Open DOS window, change your current directory to C:\MT305 and extract MicroTec components using the command

   pkunzip mt305.zip

4. Register you computer using "install" command at the command prompt (you will need the serial number from file serial_n.txt on the floppy or request one from microtec@siborg.ca)

   install /0

File "inst.pas" will be created. Please zip this file and E-mail the zipped archive to

   microtec@siborg.ca

as an attachment by E-mail. We will then register your computer and send you another "inst.pas" file. Please include the name of the contact person, phone and Fax numbers to facilitate communication should it be required. Keep a copy of the "inst.pas" at all times.

5. Unzip received "inst.pas" in the MT305 directory and run

   install /i

   This will complete the installation procedure

You may run MicroTec without registering it. In this case it will run in a demonstration mode where you can run any process simulation in a fixed domain 0.7 by 0.7 microns.

You will also be able to simulate an NMOSFET with 1 um Leff and Tox of 0.02 um. You cannot

change the transistor structure, e.g. location of electrodes, doping distribution and the domain size, but you can change the voltages, number of nodes, model parameters etc.

Without registration, for all other device simulation examples included in the distribution package you can only plot the output results and edit the input data. Do not try to run these examples because the doping distribution and geometry of the simulated device will still be that of the NMOSFET.

1.3. Quick start

Select a project in the project list window on the '**Select Project**' tab, by clicking the left mouse button on the project name, see 'Figure 2.1 Select Project tab.' on page 16. 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 several jobs using different tools, for example, 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.

To modify the project settings click on the '**Project Settings**' tab, see 'Figure 2.2 Project Settings tab.' on page 17. Another page of the main **MicroTec** window will appear showing a directives, subdirectives and parameters tree. Click on a folder symbol to open it. Double-click a parameter to edit it. If you click on a directive or subdirective with the left and then the right mouse button, a context sensitive menu appears allowing '**Delete**', '**Copy**', **'Insert Directive'** or **'Insert Subdirective'**, **'Add Subdirective'** and **'Add Parameter'**. If while a subdirective is selected you select '**Add Parameter**', a list of available parameters pops up. Select an item and click **OK**.

If you click on **'Add Subdirective'** or **'Insert Directive'** a list of available directives or subdirectives pops up. Select an item and click '**OK**'. A brief description of the directives, subdirectives and parameters is given in the selection windows. A more detailed description may be found in later chapters, where each simulator is described in detail.

The most convenient way of starting a new project is to go to the '**Select Project**' window, select an existing project similar to the desired one and then click the '**Copy**' button. A new project will be created with "(copy)" appended to the old project name. Edit the name in the '**Name**' window and click the '**Update**' button. To modify directives/parameters, switch to the "**Project Settings**" page as described above.

If you need to start a new project, type the name of the project in the '**Name**' window, select a method in the '**Method**' window and click the '**Add**' button. A project with default directive/parameter settings will be created. Change the current page to '**Project Settings**' and edit the 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 the '**2D Output**' or '**3D Output**' buttons for plotting I-V curves or 3D/colour map plots of two-dimensional distributions respectively. Click on **Plot/Add...** or **Plot/Select...** for '**2D Output**' or '**3D Output**' respectively to plot an IV-curve or a surface.

The 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 the Graphics Tools refer to Chapter 3.

2

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

The MicroTec main menu has two tabbed windows: '**Select Project**' and '**Project Settings**', that can be viewed by clicking on the named tab.

Select Project page

The first page of the MicroTec main menu, called '**Select Project**' shown in figure 2.1, comprises the following:

- Run Bar with 'Run', 'Edit', '2D Output', '3D Output', 'Help' and 'Exit' 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.
- Project Handling Bar with 'Add', 'Update', 'Copy' and 'Delete' buttons.

To select a project in the project list window on the '**Select Project**' page, click the left mouse button on a project name. The corresponding project and simulator name as well as project description will appear in the '**Name**' and '**Method**' text boxes and **'Description'** window respectively.

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

If you need to start a new project, type a project name 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 the current page to the '**Project Settings**' page and edit the parameters as described in the Section Project Settings Page on page 16.

When you start a new project, you will need to select the appropriate '**Method**' in the **'Method'**

window. The following four options are available:

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

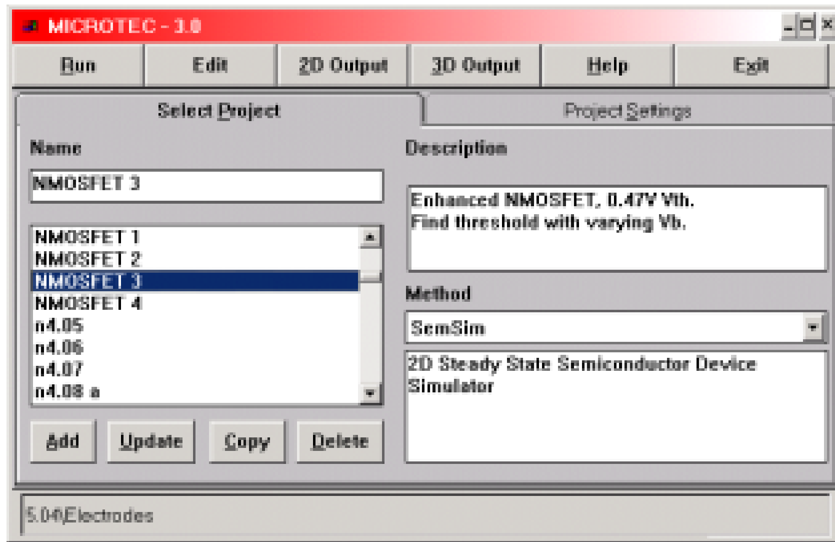

Figure 2.1 Select Project tab.

Another way of starting a new project is to copy an existing project. Select a project and click the '**Copy**' button. A new project with '(copy)' appended to it's name 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. Switch to the '**Project Settings**' page and change the parameters as needed.

To run a simulation, click the '**Run**' button. After the simulation is complete you may display the results by clicking on the '**2D Output**' or '**3D Output**' buttons 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 MicroTec Graphics: SibGraf on page 31 for more information on the **MicroTec** graphics.

Project Settings Page

To modify project settings click on the '**Project Settings**' tab. The other page of the main **MicroTec** menu will appear showing a **Project Tree** containing directives, subdirectives and parameters, as in figure 2.2. 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 with the left and then the right mouse button. A menu pops up allowing you to '**Delete**', '**Copy**', '**Insert**' or '**Add**' an entry.

If you select '**Delete**' the current entry will be deleted. If you select '**Copy**', a new copy of the current entry will be added at the end of the project tree. Selecting '**Insert**' or '**Add**' brings up a new window showing a list of entries that may be added at this stage. Select one of them and click '**OK**'. Newly added parameters are given default values. Double-clicking a parameter brings up an edit window showing the current parameter value and a brief parameter description. Edit the

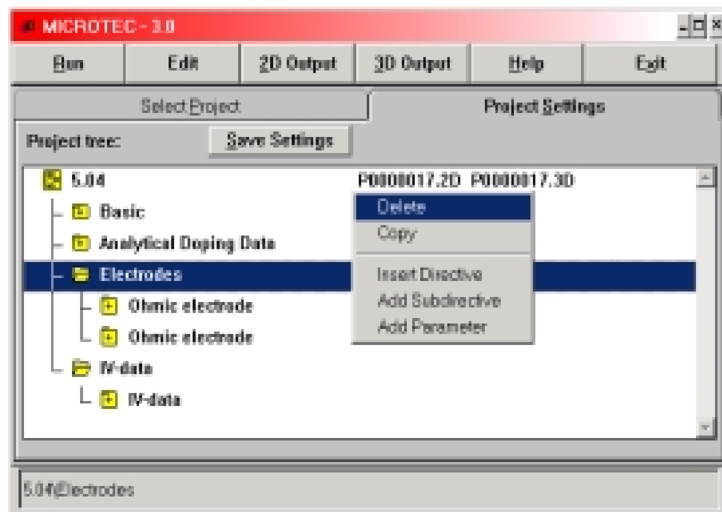

Figure 2.2 Project Settings tab. Context sensitive menu is visible.

parameter value in the text box and click '**OK**'.

There are different types of directives in **MicroTec**: unique or non-unique and mandatory or optional. For example, the '**Photogeneration**' directive is optional and unique, one may skip this directive or give it a number of subdirectives to obtain several photogeneration wells. Alternatively, the '**Basic**' directive is mandatory and unique. Any newly created project will contain all mandatory directives with parameters assigned default values. Mandatory directives cannot be deleted.

3

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 as well as several other functions. 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

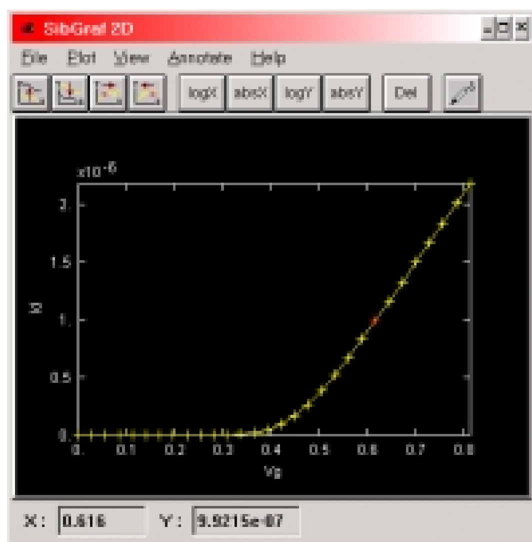

Figure 3.1 SibGraf 2D window.

This function allows you to plot any column, 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 the '**2D Output**' button in the main **MicroTec** window, a new window pops up with five menu choices: **'File'**, **'Plot'**, **'View'**, **'Annotate'** and '**Help'**. The subtopics available under these menus are described below. To zoom in on a portion of the graph use the left mouse button as described in the section titled **Zooming** below. You may also use the **Annotate** command which is also described below. The **Tool Bar** buttons allow you to change the current point and curve, switch to and from logarithmic scale and delete the current curve, shown in yellow. More information is available in the Section 2D Tool Bar on page 24.

File

Open - Open a picture file, *.mtp, previously created by this program.

Load - Load data from a file containing 2D data, e.g. IV curves. *.2d*. See "2D Data File Structure" on page 24.

Save - Save the plot to the picture file, *.mtp, 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, *.mtp. A window will be provided to allow you to choose the file name.

Clear - Clear the plot window (delete all curves in the window).

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

Import Data - Allows you to add new data from a file to the graph. The file may contain a few curves. For every curve the first line for every subset of data includes the number of points in the curve and name of the curve, followed by two columns of data for X and Y axis respectively.

Export Data - Allows you to transfer data from the graph into an ASCII file. See previous section for the file format. The file can then be imported using the Import Data command.

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

Exit - Close the window.

Plot

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 data labels are derived by appending the first letters of the **Electrode name** parameters to the predefined letters V (for voltage) and I (for current).

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 IV data and even numbers 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. The setup necessary to plot current gain, $\beta=I_C/I_B$, is shown in figure 3.2.

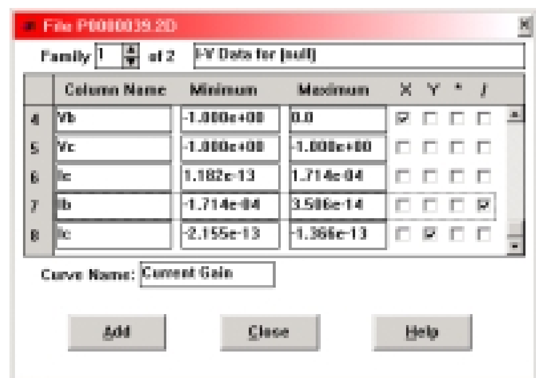

Figure 3.2 Plot/Add... menu.

The user can type the name of the curve being created into the '**Curve Name**' box. The default curve name is the name of 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. Once all the desired curves have ben added, click '**Close**' to return to the SibGraf 2D window. The data used to create a curve may be viewed later by selecting the **Curve/Source...** menu, which brings up the window shown in figure 3.3.

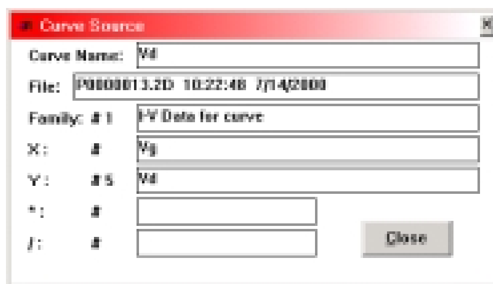

Figure 3.3 The Curve Source window.

Copy - Copy the current curve from the plot to the **SibGraf** clipboard. This feature, combined with **Paste,** is used to create compillations of curves.

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. The curve name may be changed from this window.

Line, Color, Marker - Allows changes to the corresponding attributes of the current curve.

View

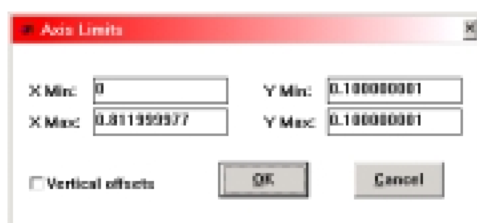

Figure 3.4 Axis Limits window.

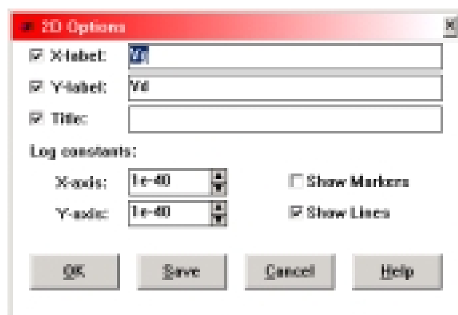

Figure 3.5 2D Options window.

Axis Limits - Allows setting the minimum and maximum values for x and y, see figure 3.4. Also allows selection of the vertical offset option. The vertical offset creates a space between the curve and the axis lines.

Options - Opens a window where the user can assign labels for horizontal and vertical axes and the title for the plot, see figure 3.5. The user can also specify the lowest value of the logarithm function corresponding to an argument approaching zero. The **Show Markers** and **Show Lines** check boxes apply to all the curves in the window. Information in this window may be saved by pressing the '**Save**' button. A file "setup.mt" will be created and the settings will be read every time a new **SibGraf** 2D window is opened.

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

Tool Bar - Switch tool bar on and off.

Status Bar - Switch status bar on and off.

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

Annotate

See the Section Annotate on page 30.

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.

2D Tool Bar

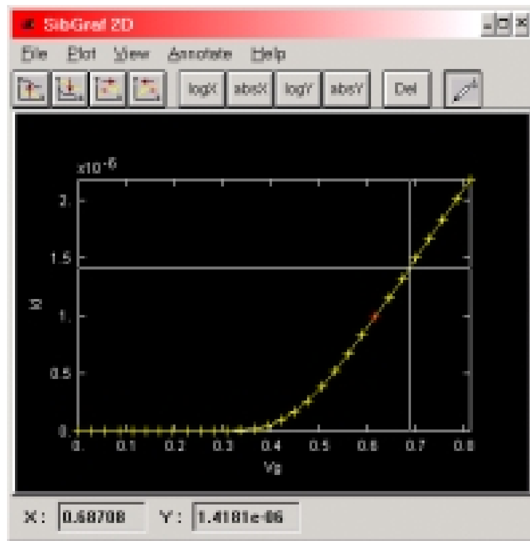

Figure 3.6 SibGraf 2D window showing

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. Each click will change the current curve to the next curve. The curves are ordered in the sequence they were added/pasted. 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 currently selected point marker on the curve. The marker of the current point is red as in figure 3.6. The buttons move the red marker to the left and right respectively. This can also be done using the left and right arrow keys on the keyboard. The x and y value of the current marker is displayed in the status bar.

The buttons **'logX'**, '**logY'**, '**absX'** and **'absY'** are used to switch to and from logarithmic and absolute scale on either the X or Y axis.

The second last button, marked **'Del'**, deletes the selected curve from the plot.

The last button switches into the tracer mode. When in tracer mode, two perpendicular lines follow the mouse along the curve. The status bar displays the x and y values of the intersection point of the two lines. This allows you to trace any part of the graph, including points that fall between markers, as in figure 3.2.

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 plotting of such quantities as current gain $\beta = I_C/I_B$, etc.

3.3. SibGraf Map/Edit Menu

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

File

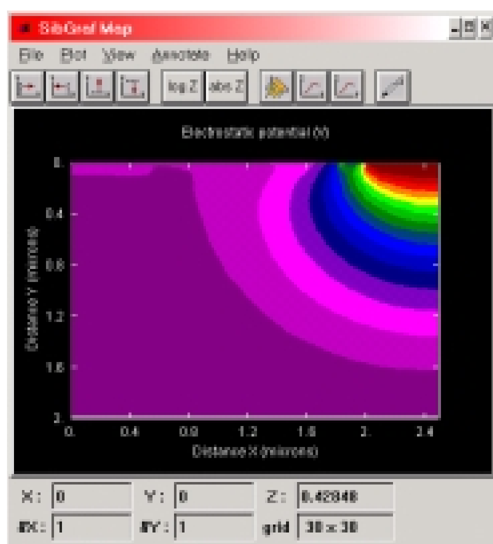

Figure 3.7 SibGraf map window.

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

Load - Load data from a file containing 2D distribution data, *.3d*.

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. *.mtm

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.

Export Data - Allows you transfer information from 'SibGraf Map' into another file.

Import Data - Allows you to add information to the 'SibGraf Map' window.

New Window - Open a new empty **SibGraf Map** window.

Exit - Close the window.

Plot

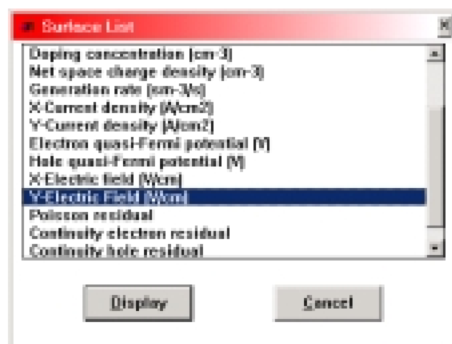

Figure 3.8 Plot/Surface... menu.

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

Select - Allows you to chose a variable to add to the SibGraf Map window, from a list of given variables. See figure 3.8.

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 - Allows you to set minimum and maximum values for the x and y (vertical and horizontal axis). See figure 3.4. The vertical offset option is not available.

Options - See Options in the Section View on page 23.

Set Contours - See the Section Map Set Contours on page 26.

Directives - Allows you to make the directives for the SibGraf Map/Edit windown visible. You can change the directives in the edit window, but not in the map window. If you are in the SibGraf Map window you may change the directives in the Projest Settings tab of the main menu. For more information see Section Directives on page 30 .

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

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

Tool bar, **Status bar**, **AutoRedraw** - Shows or hides the tool bar and status bar. Turns auto redraw on or off. With autoredraw on, the window will redraw itself automatically once a window covering it is moved.

Redraw - Redraw current plot.

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

Annotate

See section 3.5 ‘Annotate’.

Help

Index - Open a window with the help index.

About - Displays **SibGraf** info.

Map Set Contours

The ‘**Set Contours**’ subitem under the ‘**View**’ menu item of the **SibGraf Map** window opens a window where the user can assign the levels at which the contour lines are drawn for the current surface. A contour map is shown in figure 3.9.

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 an existing contour line by choosing it in the table and pressing the

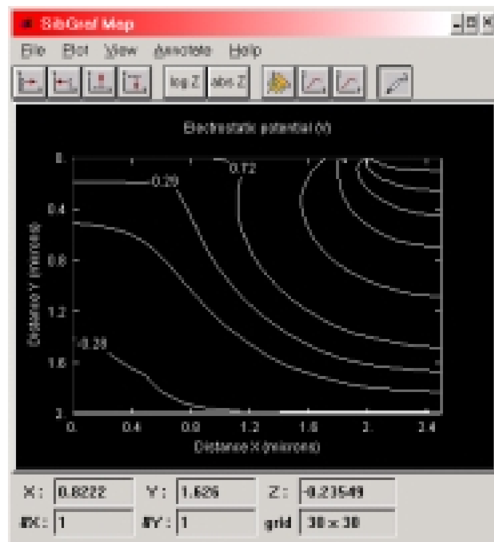

Figure 3.9 Contour map

'**Remove**' button, or modify the existing contour lines by changing their Z (or Log Z) values. The check box in front of each level value indicates whether or not the contour labels for all contours at this level are shown.

The user can also modify an 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 either this label or all contour lines at the corresponding level from the plot.

The location of a label can be changed by dragging the label with the left mouse button. If 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.

A new contour line may be added to the graph by right clicking anywhere in the graph area. The new contour line will run through the point where the mouse was clicked. Right clicking on a contour label brings up a menu allowing the deletion of the label or of the entire contour line.

Map Status Bar

The status bar is the strip at the bottom of the plot window. If probe mode is off, the first row of three numbers in the status bar show the values of the X and Y coordinates of the current cross-sections, and the Z value at the point of their intersection.

If probe mode (see below) is on, the first row of three numbers show the values of the X, Y and Z coordinates at the current mouse position.

The bottom row of numbers always show the mesh step numbers of the current X and Y cross-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 select current X and Y cross-sections. 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 button opens a **SibGraf 3D** window displaying the current function. The next two buttons are used to plot the currently selected X and Y cross-sections in a separate **SibGraf 2D** window. All subsequent cross-section plots are added to the same **SibGraf 2D** window. The last button is the '**Probe**' button. It is used to switch the probe mode on and off (see '**Map Status Bar**' above).

3.4. SibGraf 3D Output

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

File

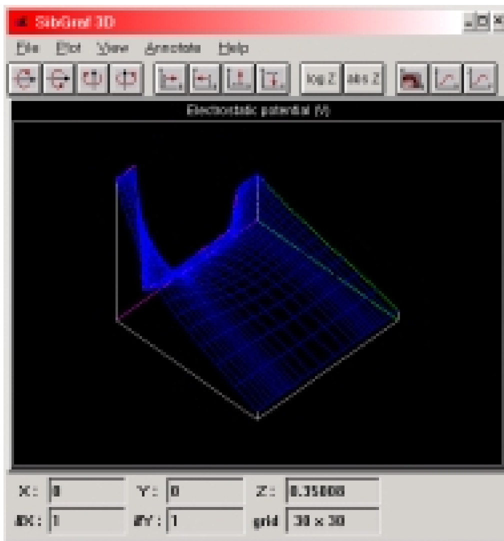

Figure 3.10 SibGraf 3D window.

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

Load - Load data from a file containing 2D distribution data, *.3d*.

Save - Save the plot to the picture file that is currently open, *.mts. 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.

Export Data - Allows you to transfer data from the graph into an ASCII file. See previous section for the file format. The file can then be imported using the Import Data command.

Import Data - Allows you to add new data from a file to the graph. The file may contain a few curves. For every curve the first line for every subset of data includes the number of points in the curve and name of the curve, followed by two columns of data for X and Y axis respectively.

New Window - Opens new Sibgraf 3D window.

Exit - Close the SibGraf 3D window.

Plot

Source - Opens a window which shows the data source for the current surface. Fields cannot be edited.

Select - gives you a variable list, figure 3.8, from which you can chose an item to plot on the graph. see figure 3.8.

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 variables that may be displayed are contained in the file and are listed in the "**Select**" window.

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 of the logarithm function corresponding to an argument approaching zero.

Tool bar, Status bar, **AutoRedraw** - allows you to make the toolbar and status bar visible or invisible. Turn auto redraw on and off. With autoredraw on, the window will redraw itself automatically once a window covering it is moved.

Redraw - Redraw current surface.

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

Annotate

See the Section Annotate on page 30.

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. If probe mode is off, the first row of three numbers in the status bar show the values of the X and Y coordinates of the current cross-sections, and the Z value at the point of their intersection.

If probe mode (see below) is on, the first row of three numbers show the values of the X, Y and Z coordinates at the current mouse position.

The bottom row of numbers always show the mesh step numbers of the 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 select different X and Y cross-sections. This can also be done by using the arrow keys on the keyboard.

The button '**Log Z**' is used to switch to and from a logarithmic scale.

The third last button is used to open a **SibGraf Map** window displaying the current function.

The last two buttons are used plot the currently selected X and Y cross-sections in a separate **SibGraf 2D** window. All subsequent cross-section plots are added to the same **SibGraf 2D** window.

3.5. Annotate

All of the **SibGraf 2D, 3D** and **Map** windows have an **Annotate** item in their main menu. Two types of annotated objects may be created: **Line** and **Text**. Annotated objects are associated with the real X and Y coordinates and not with the window or screen position. Therefore, the annotation objects move with respect to the window when windows are zoomed or resized.

When the subitem **Line** is chosen, the user can draw a line consisting of a number of straight segments. To continue a line from a point, click the left mouse button. To terminate an annotation line, click the right mouse button. To modify an existing **Annotate Line** object, first select it by clicking the left mouse button on the line. Then either the whole line or any of its nodes can be moved to the desired position with the left mouse button. Clicking 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 choose whether a 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 first select the text object, then choose the subitem **Edit** under **Annotate** in the main menu. The user can delete annotation lines or text by selecting them as the current annotated object, as described above, and then choosing the subitem **Delete** under **Annotate** in the main menu.

3.6. Zooming

The user may zoom in on a particular rectangle of any **2D, 3D** or **Map** plot. 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.

3.7. Directives

In both the **SibGraf Map** and **SibGraf Edit** windows under the View item in the main menu, there is an item called '**Directives**'. This item allows you to create directives in the window in which you are in. Directives are sections of the graph, which refer to specific sections listed in the project settings tab of the main window. You may change the directives in the **SibGraf Edit** window, by ... . Once you change the directives in the **SibGraf Edit** window and restart the program

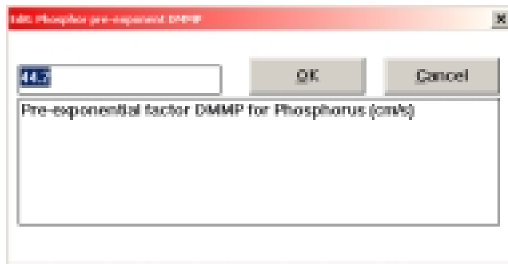

Figure 3.11

the directives will also change in the corresponding **SibGraf Map** window. To change the directives without using the **SibGraf Edit** window, simply go into the main window, into the *Project Settings* tab, there underneath the Project Tree you will find a list of names for the different directives. Double click on the directive you wish to change and a window will pop up where you can edit the directives by changing the number in the top box at press **OK** (see diagram above).

4

PROCESS SIMULATION

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

$$n = -\frac{1}{2}\left(\sum_k Z_k C_k + \sqrt{\left(\sum_k Z_k C_k\right)^2 + 4 n_i}\right) \tag{4.3}$$

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

$$E = -\frac{kT/q}{\sqrt{\left(\sum_k Z_k C_k\right)^2 + 4 n_i}} \sum_k Z_k \nabla C_k. \tag{4.5}$$

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

$$J_i = D_i \left(\nabla C_i + Z_i C_i \frac{\sum_k Z_k \nabla C_k}{\sqrt{\left(\sum_k Z_k C_k\right)^2 + 4 n_i}} \right) \tag{4.6}$$

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.

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

4.2.1. Diffusion coefficient

The diffusivity of arsenic and boron, accounting for single charged defect influence, is chosen in

the form [3,4,5]

$$D_k = D_{0k}\exp\left(\frac{-E_{0k}}{kT}\right)\left(\frac{1+\beta_k\eta}{1+\beta_k}\right) \tag{4.1}$$

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 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.

$$D_P = D_0\exp\left(\frac{-E_0}{kT}\right) + D_1\left(\frac{n}{n_i}\right)\exp\left(\frac{-E_1}{kT}\right) + D_2\left(\frac{n}{n_i}\right)^2\exp\left(\frac{-E_2}{kT}\right) \tag{4.2}$$

4.2.2. 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]

$$D_i^{ox} = D_i + \Delta D_i\left(\frac{dU}{dt}\right)^{\beta_{ox}}\exp\left(\frac{-E_{ox}}{kT}\right)\exp\left(\frac{-\Delta x}{\lambda_x}\right)\exp\left(\frac{-y}{\lambda_y}\right). \tag{4.1}$$

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].

4.2.3. Analytical oxidation model

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

$$\frac{dU}{dt} = \frac{B}{2U + A} \tag{4.1}$$

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]

$$B = P_{ox}B_o\exp\left(\frac{-E_B}{kT}\right), \quad \frac{B}{A} = OR_{ox}P_{eff}R_o\exp\left(\frac{-E_R}{kT}\right). \tag{4.2}$$

Here P_{ox} is the pressure of the oxidizing ambient in atmospheres and P_{eff} is the effective pressure 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 (4.1) leads to

$$U(t) = \sqrt{\left(U_0 + \frac{A}{2}\right)^2 + Bt} - \frac{A}{2} \tag{4.3}$$

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

$$U(x, t) = U_0 + \frac{U(t) - U_0}{2} erf\left(\frac{x - xm - \delta}{\gamma}\right) \tag{4.4}$$

with the following empirical parameters [10]

$$\delta = \frac{\delta_0 - \delta_1 T + \delta_1 \ln(U_0)}{1 + 3\chi} + (\delta_2 - \delta_3 T - \delta_4 \chi) U(t) \tag{4.5}$$

$$\gamma = \frac{\gamma_0 - \gamma_1 T + \gamma_1 \ln(U_0)}{1 + 3\chi} + (\gamma_2 - \gamma_3 T - \gamma_4 \chi) U(t) \tag{4.6}$$

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

4.2.4. 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

$$J_{ox} = C_b\left(1 - \frac{1}{\alpha_s m}\right) v_{ox} \quad (4.1)$$

where C_b is the impurity concentration in Si at the SiO_2 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 SiO_2 that is equal to 0.44.

For boron

$$m = A_{seg}\exp\left(\frac{-E_{seg}}{kT}\right), \lambda = A_{\lambda}\exp\left(\frac{-E_{\lambda}}{kT}\right). \quad (4.2)$$

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

$$J_{ox} = C_b v_{ox} \quad (4.3)$$

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]

$$J_{ox} = C_b\left(1 - \frac{1}{\alpha_s m}\right)\frac{v_{ox}\lambda}{\lambda + v_{ox}} \quad (4.4)$$

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

4.2.5. 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

$$I(y) = \frac{1}{\sqrt{2\pi}\sigma_y}\exp\left(\frac{-(y - R_p)}{2\sigma_y^2}\right) \quad (4.1)$$

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]

$$I(x, y) = \frac{I(y)}{2}\left(erf\left(\frac{x - x_r}{\sqrt{2}\sigma_x}\right) - erf\left(\frac{x - x_l}{\sqrt{2}\sigma_x}\right)\right) \quad (4.2)$$

where x_r and x_l are the coordinates of the left and the right edges of the grid cell. To obtain the final implant distribution, expression (4.2) 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/cm^2 dose and the arsenic is implanted with 100 KeV and a 10^{15} ions/cm^2 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

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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.

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:

4.6.1. SiDif Directive List

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
- **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.

Name	Default	Units	Description
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.
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	$1.0 \cdot 10^{12}$	cm^{-3}	Initial uniform phosphorus concentration.
BO	$1.0 \cdot 10^{12}$	cm^{-3}	The same parameter for boron doping.
AS	$1.0 \cdot 10^{12}$	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.
CO	10^{12}	cm^{-3}	Value of the impurity concentration considered to be a background
COMM	'Comm'	none	Comment line.

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

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.

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	$1.0 \cdot 10^{12}$	cm^{-3}	Initial uniform phosphorus concentration.
BO	$1.0 \cdot 10^{12}$	cm^{-3}	The same parameter for boron doping.
AS	$1.0 \cdot 10^{12}$	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

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

Symbol	Name	Default	Units	Description
n_{i0}	CINT	$3.873 \cdot 10^{16}$	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	BETB	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

Symbol	Name	Default	Units	Description
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
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

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	$1.66 \cdot 10^{-5}$	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	$1.44 \cdot 10^{-5}$	cm^2/s	The OED for Phosphorous (100) orientation
ΔD_i	OEP1	$5.65 \cdot 10^{-6}$	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

4.8.1. 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
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	$4.917 \cdot 10^4$	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

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

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

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

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

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	$1.0 \cdot 10^{22}$	none	The Segregation coefficient for Arsenic
A_{seg}	SEGP	$1.0 \cdot 10^{22}$	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	$1.25 \cdot 10^4$	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.

4.9.1. MOSFET fragment

Substrate with orientation <111> is doped initially with boron at 10^{15} cm^{-3}. Boron is implanted at 60 KeV and $6 \cdot 10^{11}$ ions/cm^2 in the whole region and then arsenic is implanted at 100 KeV and 10^{15} ions/cm^2 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;$
```

4.9.2. 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/cm^2. Finally the wafer is annealed at 1000 °C for 60 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;$
```

4.9.3. Fragment with LOCOS

Substrate is initially doped by boron at 10^{15} cm^{-3}. Arsenic is implanted at 200 KeV and 10^{15} ions/cm^2 in the left side of the region. Then boron is implanted at 200 KeV and 10^{14} ions/cm^2 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;$
```

4.9.4. 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;$
```

4.9.5. 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/cm^2, and annealed at 1000 °C for 1 hour in an inert ambient. Epitaxy follows for 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/cm^2 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; $
```

4.9.6. 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/cm^2 and arsenic implanted at 60 KeV and 10^{15} ions/cm^2 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;$

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 $.
- All directives after $ will be ignored.

5.3.1. 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.

5.3.2. 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.

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.

5.4.1. 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'$

5.4.2. 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'}$

5.4.3. 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';$

5.4.4. Vertical BJT with a buried layer

```
MESH:NX=200 NY=40 XX=8 YY=3.5, COMM='Planar transistor';
FRAG:X0=4. DX=1 SY=0 OV=1 IF='BUR.OUD';}
FRAG:X0=1 DX=1 SY=-1 OV=0 IF='EMIT.OUD';$
```

5.4.5. I^{2}L 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';$
```

6

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

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

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

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

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

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

$$J_p = -qp\mu_p\nabla(\psi - \chi) - qD_p\nabla p \, . \tag{6.5}$$

6.2.1. 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]

$$\chi = -\frac{\Delta E_g}{2} = \chi_0\left(ln\left(\frac{N}{N_c}\right) + \left(ln^2\left(\frac{N}{N_c}\right) + L\right)^{\frac{1}{2}}\right), \tag{6.6}$$

where $N = N_D + N_A$.

Temperature dependence of the bandgap is as follows

$$E_g(T) = E_g(0) + \frac{E_{g\alpha}T^2}{T + E_{g\beta}}. \tag{6.7}$$

Intrinsic carrier concentration is

$$n_{ie}(T) = \sqrt{N_C N_C}\exp\left(-\frac{E_g}{2kT}\right) \tag{6.8}$$

Effective density of states

$$N_C(T) = N_C(300)\left(\frac{T}{300}\right)^{3/2} \tag{6.9}$$

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

6.2.2. SRH and Auger Recombination and Impact Ionization

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

$$(R-G) = (R-G)_{SRH} + (R-G)_{Auger} - G_{av}, \tag{6.11}$$

$$(R-G)_{SRH} = \frac{np - n_{ie}^2}{(n + n_{ie})\tau_p + (p + n_{ie})\tau_n}, \tag{6.12}$$

$$(R-G)_{Auger} = (np-n_{ie}^2)(C_n n + C_p p) \ , \tag{6.13}$$

using concentration dependent lifetimes

$$\tau_n = \frac{\tau_{n0}}{\left(A_n + \left(B_n\left(\frac{N}{N_{n,\,ref}}\right) + C_n\left(\frac{N}{N_{n,\,ref}}\right)^{\alpha_n}\right)\right)} \ , \tag{6.14}$$

and an analogous expression for holes.

Impact ionization is modeled using the Chynoweth model [7]

$$G_{av} = \alpha_n|J_n| + \alpha_p|J_p|, \tag{6.15}$$

where

$$\alpha_n = a_n exp\left(\frac{-b_n|J_n|}{|(E \cdot J_n)|}\right) \text{ and } \alpha_p = a_p exp\left(\frac{-b_p|J_p|}{|(E \cdot J_p)|}\right) . \tag{6.16}$$

6.2.3. 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

$$(R-G)_{surf} = \frac{np-n_{ie}^2}{(n+n_{ie})/v_{sp} + (p+n_{ie})/v_{sn}} \ , \tag{6.17}$$

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

6.2.4. Boundary Conditions

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

$$n_0 = \sqrt{N_N^2/4 + n_{ie}^2} + N_N/2, \tag{6.18}$$

$$p_0 = \sqrt{N_N^2/4 + n_{ie}^2} - N_N/2, \quad (6.19)$$

$$\psi_0 = \frac{kT}{q}\ln\left(\frac{n_0}{n_{ie}}\right) + V_k, \quad (6.20)$$

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

$$J_{n,\nu} = qv_{sn}(n - n_{eq}), \quad (6.21)$$

$$J_{p,\nu} = -qv_{sp}(p - p_{eq}), \quad (6.22)$$

$$\psi_0 = -\Phi_B + V_k, \quad (6.23)$$

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

$$n_{eq} = n_{ie}\exp\left(\frac{q\psi_0}{kT}\right), \quad (6.24)$$

$$p_{eq} = n_{ie}\exp\left(-\frac{q\psi_0}{kT}\right). \quad (6.25)$$

On insulating segments of the boundary for current densities we have

$$J_{n,\nu} = q(R - G)_{surf}, \quad (6.26)$$

$$J_{p,\nu} = -q(R - G)_{surf}. \quad (6.27)$$

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

$$\varepsilon_1 E_{1,\nu} = \varepsilon_2 E_{2,\nu} + Q_{ss} \quad (6.28)$$

where $\varepsilon_1, \varepsilon_2$ are dielectric permittivities of the respective materials and Q_{ss} is a fixed surface charge density. For open segments of the boundary $E_{2,\nu}$ equals zero. For boundary segments underneath gate contacts the electric field is approximated by the formula

$$E_{2,\nu} = -\frac{(V_{G,eff} - \psi_s)}{h_d} \tag{6.29}$$

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.

6.2.5. Mobility Models

Several options for concentration and field dependent mobility models are available. In **BiSim** the concentration and field dependent mobility is taken in a form similar to [8]

$$\mu_{S,n}(N, E_t) = G_{surf,n}\left(\mu_n^{min} + \frac{\mu_n^{max}\left(\frac{T}{300}\right)^{\nu_n} - \mu_n^{min}}{1 + \left(\frac{T}{300}\right)^{\xi_n}\left(\frac{N}{N_{ref,n}}\right)^{\alpha_n}}\right)\left(1 + \left|\frac{E_t}{E_{cn,\mu}}\right|\right)^{-\frac{1}{2}}, \tag{6.30}$$

$$\mu_n(N, E_t, E_l) = \mu_{S,n}(N, E_t)\left(1 + \left(\frac{\mu_{S,n}E_l}{v_{sat,n}}\right)^{\beta_n}\right)^{-\frac{1}{\beta_n}}, \tag{6.31}$$

And analogous expression for holes.

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

$$\mu_n(N, E_l, E_t) = \mu_1(N, E_t)\left(1 + \frac{\left(\frac{\mu_1 E_l}{v_c}\right)^2}{G + \left(\frac{\mu_1 E_l}{v_c}\right)} + \left(\frac{\mu_1 E_l}{v_s}\right)^2\right)^{-\frac{1}{2}}, \tag{6.32}$$

$$\mu_1(N, E_t) = \mu_0\left(1 + \frac{N}{N_r + \frac{N}{S}}\right)^{-1}(1 + \alpha|E_t|)^{-\frac{1}{2}}, \tag{6.33}$$

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

$$\frac{1}{\mu} = \frac{1}{\mu_{ac}} + \frac{1}{\mu_b} + \frac{1}{\mu_{sr}}. \tag{6.34}$$

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

$$\mu_{ac}(E_t, T) = \left(B\frac{T}{E_t} + \frac{C}{E_t^{\frac{1}{3}}}\right); \tag{6.35}$$

$$\mu_b(N, T) = \mu_0 + \frac{\mu_{max(T)} - \mu_0}{1 + \left(\frac{N}{C_r}\right)^{\alpha}} - \frac{\mu_1}{1 + \left(\frac{C_s}{N}\right)^{\beta}}; \tag{6.36}$$

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.

We transform to dimensionless variables [15]

$$\psi_{new} = \frac{\psi}{kT},\ x_{new} = \frac{x}{l_D},\ n_{new} = \frac{n}{n_i} \tag{6.37}$$

where l_D is the intrinsic Debye length. Retaining the "old" notation for the "new" dimensionless variables we obtain

$$\nabla^2\psi = n - p - N_D + N_A , \qquad (6.38)$$

$$\nabla J_n = (R - G) , \qquad (6.39)$$

$$-\nabla J_p = (R - G) . \qquad (6.40)$$

6.3.6. Finite-Difference Scheme

In the two-dimensional case, standard discretization of (4-6) using a central-difference scheme for the Poisson equation and the Scharfetter-Gummel approximation [11] for the current densities gives (see e.g. [15]),

$$(\Delta_{rh}\psi)_{i,j} = h_i^* r_j^* (n(\psi)_{i,j} - p(\psi)_{i,j} - (N_D - N_A)_{i,j}) , \qquad (6.41)$$

$$(\Lambda_n(\psi)n)_{i,j} = h_i^* r_j^* (R - G)_{i,j} , \qquad (6.42)$$

$$(\Lambda_p(\psi)p)_{i,j} = h_i^* r_j^* (R - G)_{i,j} . \qquad (6.43)$$

The subscripts i, j number the grid nodes, $h_i = x_{i+1} - x_i$ and $r_j = r_{j+1} - r_j$ are the sizes of the space steps, τ is the time step,

$h_i^* = \frac{(h_i + h_{i-1})}{2}$, $r_j^* = \frac{(r_j + r_{j-1})}{2}$, Δ_{rh} is the discretized Laplace operator

$$(\Delta_{rh}\psi)_{i,j} = \frac{r_j^*}{h_i}(\psi_{i+1,j} - \psi_{i,j}) - \frac{r_j^*}{h_{i-1}}(\psi_{i,j} - \psi_{i-1,j}) + \frac{h_i^*}{r_j}(\psi_{i,j+1} - \psi_{i,j}) - \frac{h_i^*}{r_{j-1}}(\psi_{i,j} - \psi_{i,j-1}) \qquad (6.44)$$

Λ_n, Λ_p represent the operators for the discretized continuity equations for electrons and holes respectively

$$(\Lambda_n(\psi)n)_{i,j} = a_{i,j}^n n_{i-1,j} + b_{i,j}^n n_{i,j-1} - e_{i,j}^n n_{i,j} + c_{i,j}^n n_{i+1,j} + d_{i,j}^n n_{i,j+1} , \qquad (6.45)$$

$$(\Lambda_p(\psi)p)_{i,j} = a^p_{i,j}p_{i-1,j} + b^p_{i,j}p_{i,j-1} - e^p_{i,j}p_{i,j} + c^p_{i,j}p_{i+1,j} + d^p_{i,j}p_{i,j+1} \quad . \tag{6.46}$$

To reduce the number of formulae and indices involved we introduce the "discretized Bernoulli functions". For electrons

$$B_n(\Delta\psi_i) \equiv B_n(\psi_{i+1,j} - \psi_{i,j}) = \mu^n_{i+\frac{1}{2},j}\frac{r^*_j}{h_i}\frac{\Delta\psi_i}{(exp(\Delta\psi_i) - 1)} \equiv \mu^n_{i+\frac{1}{2},j}\frac{r^*_j}{h_i}B(\Delta\psi_i) \quad , \tag{6.47}$$

$$B_n(\Delta\psi_j) \equiv B_n(\psi_{i,j+1} - \psi_{i,j}) = \mu^n_{i,j+\frac{1}{2}}\frac{h^*_i}{r_j}\frac{\Delta\psi_j}{(exp(\Delta\psi_j) - 1)} \equiv \mu^n_{i,j+\frac{1}{2}}\frac{h^*_i}{r_j}B(\Delta\psi_j) \quad . \tag{6.48}$$

where $\mu^n_{i+\frac{1}{2},j}$ and $\mu^n_{i,j+\frac{1}{2}}$ are the electron mobilities at the midpoints

between the mesh nodes, and $B(\Delta\psi_i) = \dfrac{\Delta\psi_i}{(exp(\Delta\psi_i) - 1)}$ is the conventional Bernoulli function.

Corresponding expressions for holes have exactly the same form with the substitution $\mu^p \rightarrow \mu^n$.

The expressions for the matrix coefficients of Λ_n, Λ_p now take a very simple form

$$a^n_{i,j} = B_n(-\Delta\psi_{i-1} + \Delta\chi_{i-1}) \ , \ b^n_{i,j} = B_n(-\Delta\psi_{j-1} + \Delta\chi_{j-1}) \ , \tag{6.49}$$

$$c^n_{i,j} = B_n(\Delta\psi_i - \Delta\chi_i) \ , \ d^n_{i,j} = B_n(\Delta\psi_j - \Delta\chi_j) \ , \tag{6.50}$$

$$a^p_{i,j} = B_p(\Delta\psi_{i-1} - \Delta\chi_{i-1}) \ , \ b^p_{i,j} = B_p(\Delta\psi_{j-1} - \Delta\chi_{j-1}) \ , \tag{6.51}$$

$$c^p_{i,j} = B_p(-\Delta\psi_i + \Delta\chi_i) \ , \ d^p_{i,j} = B_p(-\Delta\psi_j + \Delta\chi_j) \ , \tag{6.52}$$

and for $e^n_{i,j}$, $e^p_{i,j}$ the relation

$$e_{i,j} = a_{i+1,j} + b_{i,j+1} + c_{i-1,j} + d_{i,j-1} \tag{6.53}$$

is valid.

The conventional Gummel decoupled scheme converges slowly in the case of high injection level. To improve the convergence a modified linearization of the discretized Poisson equation [3] has been introduced described in the following section. Initial guess strategy which is particularly important for the code efficiency and stability is also described below.

6.3.7. Modified linearization of the discretized Poisson equation

The discretized Poisson equation is

$$(\Delta_{rh}\psi^k)_{i,j} = h_i r_j (n(\psi^k)_{i,j} - p(\psi^k)_{i,j} - (N_D - N_A)_{i,j}) \quad . \tag{6.54}$$

The superscript k is the iteration number. The dependencies of $n(\psi^k)_{i,j}$ and $p(\psi^k)_{i,j}$ upon ψ^k are shown explicitly in equation (6.54) to emphasize the nonlinear nature of the Poisson equation. Failure to correctly take into account this non-linearity leads to divergence, when sequentially solving the Poisson and continuity equations. Gummel [14] used an exponential dependence $n = exp(\psi - \varphi_n)$, $p = exp(\varphi_p - \psi)$ to linearize equation (6.54). The quasi-Fermi potentials φ_n and φ_p were considered fixed when iterating over the non-linear equation (6.54) and φ_n, φ_p were updated only when solving the continuity equation. This is a good approximation when one has a rather accurate initial guess for φ_n, φ_p. However when high injection occurs the Gummel iterations converge slowly.

We propose using the discretized continuity equation to estimate the

derivatives $\frac{dn}{d\psi}$ and $\frac{dp}{d\psi}$. We use the expressions $n = exp(\psi - \varphi_n(\psi))$,

$p = exp(\varphi_p(\psi) - \psi)$, where the dependencies $\varphi_n(\psi), \varphi_p(\psi)$ are estimated from the discretized continuity equation. The changes in $\varphi_n(\psi), \varphi_p(\psi)$ caused by the changing ψ value during the Poisson iteration are estimated. The approach leads to the following form for the linearized discretized Poisson equation (6.54)

$$\frac{(\Delta_{rh}\psi^k)_{i,j}}{h_i^* r_j^*} = n(\psi_{i,j}^{k-1}) - p(\psi_{i,j}^{k-1}) - (N_D - N_A)_{i,j} + (\alpha_{i,j}^n n(\psi_{i,j}^{k-1}) + \alpha_{i,j}^p p(\psi_{i,j}^{k-1}))(\psi_{i,j}^k - \psi_{i,j}^{k-1}) \tag{6.55}$$

where

$\alpha_{i,j}^{n} = \dfrac{d}{d\psi_{i,j}} ln(n_{i,j})$ and $\alpha_{i,j}^{n} = \dfrac{d}{d\psi_{i,j}} ln(n_{i,j})$.

Obviously $\alpha_{i,j}^{p} = \alpha_{i,j}^{n} = 1$ when, $\dfrac{d\varphi_{n,i,j}}{d\psi_{i,j}} = \dfrac{d\varphi_{p,i,j}}{d\psi_{i,j}} = 0$, and in this case we arrive

at the conventional Gummel scheme. Note also that the expressions for updating the carrier concentrations become

$n(\psi_{i,j}^{k}) = n(\psi_{i,j}^{k-1}) exp(\alpha_{i,j}^{n}(\psi_{i,j}^{k} - \psi_{i,j}^{k-1}))$ and

$p(\psi_{i,j}^{k}) = p(\psi_{i,j}^{k-1}) exp(-\alpha_{i,j}^{p}(\psi_{i,j}^{k} - \psi_{i,j}^{k-1}))$.

The discretized continuity equations are used to estimate α_n and α_p. We express $n_{i,j}$ and $p_{i,j}$ using equations (8-11) obtaining

$$n_{i,j} = \frac{a_{i,j}^{n} n_{i-1,j} + b_{i,j}^{n} n_{i,j-1} + c_{i,j}^{n} n_{i+1,j} + d_{i,j}^{n} n_{i,j+1}}{e_{i,j}^{n}}, \qquad (6.56)$$

$$p_{i,j} = \frac{a_{i,j}^{p} p_{i-1,j} + b_{i,j}^{p} p_{i,j-1} + c_{i,j}^{p} p_{i+1,j} + d_{i,j}^{p} p_{i,j+1}}{e_{i,j}^{p}}, \qquad (6.57)$$

where we have neglected the generation-recombination term $(R - G)_{i,j}$.

We use equations (19,20) to evaluate α_n and α_p from their derivatives with respect to $\psi_{i,j}$.

The assumptions about the carrier density dependencies on ψ are particularly important. As shown in [3], choosing an exponential dependence we arrive at the generalized Gummel linearization (GGL), while assuming the densities to be independent of ψ we arrive at the generalized Mock scheme (GMS) [16]. GGL coincides with the conventional Gummel linearization if the difference of the quasi-Fermi potentials at the adjacent mesh nodes vanishes.

Introduction of the coefficients α_n, α_p may speed-up the convergence of Gummel iterations by up to 7 times in the case of high injection [3].

6.3.8. Initial guess strategy

The total current continuity equation is used for the evaluation of the initial guess and it is essentially a combination of Eqs.(5,6)

$$\nabla(J_n + J_p) = 0 .$$

The operator form of the discretized equation (21) is

$$\Lambda_n(\psi^k)n^k + \Lambda_p(\psi^k)p^k = 0 ,$$

where $\Lambda_n(\psi^k)$, $\Lambda_p(\psi^k)$ and Δ_{rh} are respectively the finite difference operators of the continuity and Poisson equations. The superscript k is the iteration number and ψ_0 is the electrostatic potential from the previous bias.

Linearization of (22) with respect to $\delta\psi^k = \psi^k - \psi^{k-1}$ and the assumption that the carrier concentrations n and p remain unchanged give

$$\Lambda(\psi^{k-1}, n^{k-1}, p^{k-1})\delta\psi^k = \Lambda_n(\psi^k)n^k + \Lambda_p(\psi^k)p^k$$

where $\Lambda(\psi^k, n^k, p^k)$ is the derivative of $\Lambda_n(\psi^k)n^k + \Lambda_p(\psi^k)p^k$ with respect to ψ^k

$$(\Lambda(\psi, n, p)\delta\psi)_{i,j} = a^{\lambda}_{i,j}\delta\psi_{i-1,j} + b^{\lambda}_{i,j}\delta\psi_{i,j-1} - e^{\lambda}_{i,j}\delta\psi_{i,j} + c^{\lambda}_{i,j}\delta\psi_{i+1,j} + d^{\lambda}_{i,j}\delta\psi_{i,j+1}$$

To simplify the formulae and to reduce the number of indexes involved it is convenient to introduce the "discretized derivatives of the Bernoulli function" for electrons (again for holes the substitution $\mu^p \to \mu^n$ should be made)

$$F_n(\Delta\psi_i) \equiv F_n(\psi_{i+1,j} - \psi_{i,j}) \equiv \mu^n_{i+\frac{1}{2},j}\frac{r_j^*}{h_i}F(\Delta\psi_i) ,$$

$$F_n(\Delta\psi_j) \equiv F_n(\psi_{i,j+1} - \psi_{i,j}) \equiv \mu^n_{i,j+\frac{1}{2}}\frac{h_i^*}{r_j}F(\Delta\psi_j) ,$$

where $F(x) = -\frac{d}{dx}B(x) = \frac{1 - exp(x) + x \cdot exp(x)}{(exp(x) - 1)^2}$ is the derivative of the Bernoulli function.

Thus we have the following expressions for the matrix elements of $\Lambda(\psi, n, p)$

$$a^{\lambda n}_{i,j} = F_n(-\Delta\psi_{i-1} + \Delta\chi_{i-1})n_{i-1,j} + F_n(\Delta\psi_{i-1} - \Delta\chi_{i-1})n_{i,j} ,$$

$$a^{\lambda p}_{i,j} = F_p(\Delta\psi_{i-1} - \Delta\chi_{i-1})p_{i-1,j} + F_p(-\Delta\psi_{i-1} + \Delta\chi_{i-1})p_{i,j} ,$$

$$b^{\lambda n}_{i,j} = F_n(-\Delta\psi_{j-1} + \Delta\chi_{j-1})n_{i,j-1} + F_n(\Delta\psi_{j-1} - \Delta\chi_{j-1})n_{i,j} ,$$

$$b_{i,j}^{\lambda p} = F_p(\Delta\psi_{j-1} - \Delta\chi_{j-1})p_{i,j-1} + F_p(-\Delta\psi_{i-1} + \Delta\chi_{i-1})p_{i,j} ,$$

$$c_{i,j}^{\lambda n} = F_n(-\Delta\psi_i + \Delta\chi_i)n_{i,j} + F_n(\Delta\psi_i - \Delta\chi_i)n_{i+1,j} ,$$

$$c_{i,j}^{\lambda p} = F_p(\Delta\psi_i - \Delta\chi_i)p_{i,j} + F_p(-\Delta\psi_i + \Delta\chi_i)p_{i+1,j} ,$$

$$d_{i,j}^{\lambda n} = F_n(-\Delta\psi_j + \Delta\chi_j)n_{i,j} + F_n(\Delta\psi_j - \Delta\chi_j)n_{i,j+1} ,$$

$$d_{i,j}^{\lambda p} = F_p(\Delta\psi_j - \Delta\chi_j)p_{i,j} + F_p(-\Delta\psi_j + \Delta\chi_j)p_{i,j+1} ,$$

$$a_{i,j}^{\lambda} = a_{i,j}^{\lambda n} + a_{i,j}^{\lambda p}; b_{i,j}^{\lambda} = b_{i,j}^{\lambda n} + b_{i,j}^{\lambda p}; c_{i,j}^{\lambda} = c_{i,j}^{\lambda n} + c_{i,j}^{\lambda p}; d_{i,j}^{\lambda p} = d_{i,j}^{\lambda n} + d_{i,j}^{\lambda p};$$

$$e_{i,j}^{\lambda} = a_{i,j}^{\lambda} + b_{i,j}^{\lambda} + c_{i,j}^{\lambda} + d_{i,j}^{\lambda}.$$

According to [16] the initial guess for the potential is obtained by solving Eq.(22) with $\psi^{k-1}, n^{k-1}, p^{k-1}$ taken from the previous bias. When the carrier concentrations are fixed (i.e. $n = exp(\psi - \varphi_n), p = exp(\varphi_p - \psi)$ and hence $(\psi - \varphi_n), (\varphi_p - \psi)$ are fixed), updating of the potential leads to implicit quasi-Fermi potential updates.

6.4. References

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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.

6.6.9. SemSim list of directives

Directive/subdirective tree looks as follows.

#BAS: Basic directives

- **MESH:** Mesh and domain parameters
- **SOLV:** 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 bandgap

- **PERM**: Dielectric permittivity
- **WORK**: Workfunction

#MOB: Mobility models

- **CONM**: Constant mobility
- **YAMA**: Yamaguchi mobility
- **LOMB**: Lombardi mobility
- **BIPO**: 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

6.6.10. #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.
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.

6.6.11. #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
DOP	$1 \cdot 10^{18}$	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.

Name	Default	Units	Description
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.

6.6.12. #OXI: Oxide

This directive may include up to 20 **OXID** subdirectives. Each rectangular region is defined by one **OXID** subdirective.

OXID: Oxide region

Name	Default	Units	Description
COMM	'Name'	none	Region description
PERM	3.8	no units	Oxide permittivity
XOXL	0	um	Left edge of the oxide well.
XOXR	1	um	Right edge of the oxide well.
YOXT	0	um	Top of the oxide well.
YOXB	1	um	Bottom of the oxide well.
QOXL	0	cm^{-2}	Qss at the left edge of the oxide well.
QOXR	0	cm^{-2}	Qss at the right edge of the oxide well.
QOXT	0	cm^{-2}	Qss at the top of the oxide well.
QOXB	0	cm^{-2}	Qss at the bottom of the oxide well.

6.6.13. #REM: Remesh

This directive may include up to 20 **REME** subdirectives. Each rectangular region is defined by one **REME** subdirective.

REME: Remesh region

Name	Default	Units	Description
COMM	'Name'	none	Region name
NXRM	5	no units	Number of extra X-nodes in the region
NYRM	5	no units	Number of extra Y-nodes in the region
XRML	0	um	Left edge of the remesh well.
XRMR	1	um	Right edge of the remesh well.
YRMT	0	um	Top of the remesh well.
YRMB	1	um	Bottom of the remesh well.

6.6.14. #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	$1 \cdot 10^{-15}$	cm/s	Electron recombination velocity under the gate.
VSP	$1 \cdot 10^{-15}$	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.

Name	Default	Units	Description
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	$1 \cdot 10^5$	cm/s	Electron recombination velocity at the interface.
VSP	$1 \cdot 10^5$	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.

6.6.15. #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.
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.

6.6.16. #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	$4.73 \cdot 10^{-4}$	eV	Value of Alpha in the formula for the bandgap width
$E_{g\beta}$	EGBE	$6.36 \cdot 10^{2}$	^{o} K	Temperature correction term in the formula for the bandgap width
$N_C(300)$	ENC3	$2.8 \cdot 10^{19}$	cm^{-3}	The semiconductor conduction band density of states
$N_V(300)$	ENV3	$1.04 \cdot 10^{19}$	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	$1.0 \cdot 10^{17}$	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

6.6.17. #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	$cm^2/V{\cdot}s$	Constant mobility for electrons
$\mu_{p,0}$	UMP0	500	$cm^2/V{\cdot}s$	Constant mobility for holes

YAMA: Yamaguchi mobility model

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

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

Symbol	Name	Default	Units	Description
μ_{n0}	UMN0	$1.4{\cdot}10^3$	cm^2/Vs	Maximum electron mobility
S_n	SN	350.0	none	Doping concentration factor for electrons
N_{rn}	RSN	$3.0{\cdot}10^{16}$	cm^{-3}	Reference doping concentration for electrons

Symbol	Name	Default	Units	Description
α_n	ALN	$1.54 \cdot 10^{-5}$	cm/V	Perpendicular electric field factor for electrons
v_{sn}	VSN	$1.036 \cdot 10^{7}$	cm/s	Saturation velocity for electrons
G_n	GN	8.8	none	Parallel electric filed factor for electrons
v_{cn}	VCN	$4.9 \cdot 10^{6}$	cm/s	Phonon velocity fitting parameter
μ_{p0}	UMP0	480.0	$cm^2/V \cdot s$	Maximum hole mobility
S_p	SP	81.0	none	Doping concentration factor for electrons
N_{rp}	RSP	$4.0 \cdot 10^{16}$	cm^{-3}	Reference doping concentration for holes
α_p	ALP	$5.35 \cdot 10^{-5}$	cm/V	Perpendicular electric field factor for holes
v_{sp}	VSP	$1.2 \cdot 10^{7}$	cm/s	Saturation velocity for holes
G_p	GP	1.6	none	Parallel electric filed factor for holes
v_{cp}	VCP	$2.928 \cdot 10^{6}$	cm/s	Phonon velocity fitting parameter

LOMB: Lombardi surface mobility model

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

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

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

Symbol	Name	Default	Units	Description
B	BN	$4.75 \cdot 10^{7}$	cm/s	Fitting parameter for perpendicular electric filed
C_o	C0N	$1.74 \cdot 10^{5}$		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	$cm^2/V \cdot s$	Minimum hole mobility
μ_{max}	UMAN	$1.42 \cdot 10^{3}$	$cm^2/V \cdot s$	Maximum hole mobility
μ_1	ULN	43.4	$cm^2/V \cdot s$	Concentration correction term
C_r	CRN	$9.68 \cdot 10^{16}$	cm^{-3}	Critical doping concentration
C_s	CSN	$3.43 \cdot 10^{20}$	cm^{-3}	Critical doping concentration in the correction term
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	$5.82 \cdot 10^{14}$	V/s	Acoustic term parameter
$\beta_{sat,\,n}$	BESN	2.0	none	Exponent in the saturation velocity
$v_{sat,\,n}$	VSAN	$1.07 \cdot 10^{7}$	cm/s	Saturation velocity

Analogous parameters for holes (note that expression for μ_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
B	BP	$9.93 \cdot 10^{7}$	cm/s	Fitting parameter for perpendicular electric filed
C_o	C0P	$8.84 \cdot 10^{5}$		Fitting parameter for perpendicular electric filed and doping concentration
θ	CPOP	$3.17 \cdot 10^{-2}$	none	Exponent of the doping concentration parameter
μ_0	U0P	44.9	$cm^2/V \cdot s$	Minimum electron mobility
μ_{max}	UMAP	470	$cm^2/V \cdot s$	Maximum electron mobility
μ_1	ULP	29	$cm^2/V \cdot s$	Concentration correction term
C_r	CRP	$2.23 \cdot 10^{17}$	cm^{-3}	Critical doping concentration
C_s	CSP	$6.10 \cdot 10^{20}$	cm^{-3}	Critical doping concentration in the correction term
P_c	PCP	$9.23 \cdot 10^{16}$	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	$2.05 \cdot 10^{14}$	V/s	Acoustic term parameter
$\beta_{sat,\,p}$	BESP	1.0	none	Exponent in the saturation velocity
$v_{sat,\,p}$	VSAP	$1.07 \cdot 10^{7}$	cm/s	Saturation velocity

BIPO: Bipolar mobility model

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

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

Symbol	Name	Default	Units	Description
$\mu_{n,\,min}$	UMNM	55.2	$cm^2/V{\cdot}s$	Minimum electron mobility
$\mu_{n,\,max}$	UMNX	1430	$cm^2/V{\cdot}s$	Maximum electron mobility
$N_{ref,\,n}$	CRFN	$1.07{\cdot}10^{17}$	cm^{-3}	Reference impurity concentration for electrons
E_{cmn}	ECNM	$6.49{\cdot}10^4$	V/cm	Critical electric field in the perpendicular electric field mobility for electrons
$v_{sat,\,n}$	VSTN	$1.07{\cdot}10^7$	cm/s	Electron saturation velocity
ν_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	$cm^2/V{\cdot}s$	Minimum hole mobility
$\mu_{p,\,max}$	UMPX	479	$cm^2/V{\cdot}s$	Maximum hole mobility
$N_{ref,\,p}$	CRFP	$1.6{\cdot}10^{17}$	cm^{-3}	Reference impurity concentration for holes
E_{cmp}	ECPM	$1.87{\cdot}10^4$	V/cm	Critical electric field in the perpendicular electric field mobility for holes
$v_{sat,\,p}$	VSTP	$1.06{\cdot}10^7$	cm/s	Hole saturation velocity
ν_p	UNP	-2.2	none	Exponent of normalized temperature in the numerator for holes

Symbol	Name	Default	Units	Description
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	BETP	1.0	none	Exponent used in the field-dependent hole mobility for parallel electric field

6.6.18. #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	$1.0 \cdot 10^{-7}$	s	Life time for electrons
$N_{SRH,\,n}$	NSRN	$5.0 \cdot 10^{16}$	cm^{-3}	Concentration parameter
$A_{SRH,\,n}$	ANSR	1.0	none	parameter

Symbol	Name	Default	Units	Description
$B_{SRH,n}$	BNSR	1.0	none	parameter
$C_{SRH,n}$	CNSR	0.0	none	parameter
$\alpha_{SRH,n}$	EN	2.0	none	parameter
τ_{p0}	TAUP	$1.0 \cdot 10^{-7}$	s	Life time for holes
$N_{SRH,p}$	NSRP	$5.0 \cdot 10^{16}$	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	$2.8 \cdot 10^{-31}$	cm^6/s	Auger recombination coefficient
$C_{Aug,p}$	AUGP	$9.9 \cdot 10^{-32}$	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	$1 \cdot 10^{-10}$	cm/s	Surface recombination velocity for electrons

Symbol	Name	Default	Units	Description
v_{sp}	VSRP	$1 \cdot 10^{-10}$	cm/s	Surface recombination velocity for electrons

RADI: Radiative recombination parameters

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

Symbol	Name	Default	Units	Description
B	RATE	$1 \cdot 10^{-14}$	cm^{-3}/s	Radiative recombination coefficient

6.6.19. #IMP: Impact Ionization

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

IONE: Impact ionization exponent

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

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	$4.0 \cdot 10^5$	V/cm	Electric field range E_0-E_1 for electrons
E_2	EN2	$6.0 \cdot 10^5$	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	$1.4 \cdot 10^6$	V/cm	Field exponent for electrons in E_0 - E_1

Symbol	Name	Default	Units	Description
$b^2{}_n$	BN2	$1.4 \cdot 10^6$	V/cm	Field exponent for electrons in E_1 - E_2
$b^3{}_n$	BN3	$1.4 \cdot 10^6$	V/cm	Field exponent for electrons in E_2 -
E_0	EP0	0.0	V/cm	Electric field range for holes
E_1	EP1	$6.07 \cdot 10^5$	V/cm	Electric field range for holes
E_2	EP2	$6.07 \cdot 10^5$	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	$2.09 \cdot 10^6$	V/cm	Field exponent for holes in E_0 - E_1
$b^2{}_p$	BP2	$1.4 \cdot 10^6$	V/cm	Field exponent for holes in E_1 - E_2
$b^3{}_p$	BP3	$1.4 \cdot 10^6$	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
$a^0{}_n$	AN0	0.0	1/cm	Ioniz.coef.for elect. in range 0 - E_0
$a^1{}_n$	AN1	$7.0 \cdot 10^5$	1/cm	Ioniz.coef.for elect. in range E_0 - E_1
$a^2{}_n$	AN2	$7.0 \cdot 10^5$	1/cm	Ioniz.coef.for elect. in range E_1 - E_2
$a^3{}_n$	AN3	$7.0 \cdot 10^5$	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	$1.3 \cdot 10^6$	1/cm	Ioniz.coef.for holes in range E_0 - E_1
$a^2{}_p$	AP2	$4.4 \cdot 10^5$	1/cm	Ioniz.coef.for holes in range E_1 - E_2
$a^3{}_p$	AP3	$4.4 \cdot 10^5$	1/cm	Ioniz.coef.for holes in range E_2 - infinity

6.6.20. #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	$1 \cdot 10^{20}$	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.

6.6.21. #OXI: Oxide region

This directive may include up to 20 **OXID** subdirectives. Each rectangular region is defined by one **OXID** subdirective.

OXID: Oxide region

Name	Default	Units	Description
COMM	‘Name’	none	Region description
PERM	3.8	no units	Oxide permittivity
XOXL	0	um	Left edge of the oxide well.
XOXR	1	um	Right edge of the oxide well.
YOXT	0	um	Top of the oxide well.
YOXB	1	um	Bottom of the oxide well.
QOXL	0	cm^{-2}	Qss at the left edge of the oxide well.

Name	Default	Units	Description
QOXR	0	cm^{-2}	Qss at the right edge of the oxide well.
QOXT	0	cm^{-2}	Qss at the top of the oxide well.
QOXB	0	cm^{-2}	Qss at the bottom of the oxide well.

6.6.22. #REM: Remesh region

This directive may include up to 20 **REME** subdirectives. Each rectangular region is defined by one **REME** subdirective with the following parameters.

REME: Remesh region

Name	Default	Units	Description
COMM	'Name'	none	Region name
NXRM	5	no units	Number of extra X-nodes in the region
NYRM	5	no units	Number of extra Y-nodes in the region
XRML	0	um	Left edge of the remesh well.
XRMR	1	um	Right edge of the remesh well.
YRMT	0	um	Top of the remesh well.
YRMB	1	um	Bottom of the remesh well.

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