Part 9

Advanced Calibration
# Part 9 – Advanced Calibration

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1.1 About this manual

The ISE Calibration Group works continually on improving the simulation models and optimizing the model parameters for the latest technology nodes. This effort is based on a long-standing experience of model calibration for customers and a comprehensive, growing database of state-of-the-art secondary ion mass spectroscopy (SIMS) profiles. As part of the process simulator DIOS, ISE provides a set of parameters that have been calibrated to deep submicron CMOS technology. With these parameters, the accuracy of DIOS simulation results is significantly improved for many fabrication processes such as ion implantation, ultra shallow junction (USJ) formation, surface dose loss, and channel and halo dopant diffusion.

1.2 Scope of the manual

This documentation is a user and reference manual for the Advanced Calibration of the process simulator DIOS:

- Chapter 2 explains how the Advanced Calibration is used. It is recommended to read this section. Section 2.2.3 on page 9.5 contains an example for the correct use of the parameter files.
- Chapter 3 details the meaning of all models and parameters used in the Advanced Calibration files. Basically, the same information can also be found in the DIOS manual.
- Chapter 4 summarizes the calibration strategy used by ISE. This would be of interest to experienced TCAD users, who want to perform their own calibration or customization of process simulation parameters.
- Chapter 5 discusses the limitations and the accuracy of the Advanced Calibration. It provides an overview of which process simulation tasks a high accuracy can be expected, and which models have not been considered in the Advanced Calibration.
- Chapter 6 summarizes the file names of the new implantation lookup tables.

1.3 Parameter files

All parameters are contained in two DIOS parameter files, which can be loaded into DIOS using the command lines:

@calib_par_85_CTRIM.cmd

or:

@calib_par_85_tables.cmd

These files are located in:

$ISEROOT/tcad/$ISERELEASE/lib/dioslib/calib_par_85_CTRIM.cmd
$ISEROOT/tcad/$ISERELEASE/lib/dioslib/calib_par_85_tables.cmd
Both files will set the same parameters for diffusion. The difference is that the first parameter file uses the Monte Carlo simulator Crystal-TRIM for implantation (which is more accurate in 2D structures, where lateral straggling is important), and the second uses the new ISE implantation tables (which require less CPU time). It is possible to use both parameter files within the same DIOS input file.

### 1.4 Pair diffusion model

The parameters used in `calib_par_85_CTRIM.cmd` and `calib_par_85_tables.cmd` are calibrated only for the DIOS pair diffusion model. This model is recommended for deep submicron CMOS or SOI devices. For simpler diffusion models (for example, the equilibrium diffusion model, which is frequently used in the process simulation of power devices), the calibrated diffusion parameters are not applicable and must not be loaded.

However, even when working with a simpler diffusion model, the parameters of the Advanced Calibration can still be used for calculating the dopant distribution after implantations. The easiest way to do this is by direct insertion of the corresponding parameters in the implantation statements. For Monte Carlo implantation, these parameters are listed in Table 9.5 on page 9.11 and, for analytical implantation, it is recommended to use the tables listed in Table 9.12 on page 9.59.

### 1.5 Terms and conventions

<table>
<thead>
<tr>
<th>Term</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Click</td>
<td>Using the mouse, point to an item, press and release the left mouse button.</td>
</tr>
<tr>
<td>Double-click</td>
<td>Using the mouse, point to an item and in rapid succession, click the left mouse button twice.</td>
</tr>
<tr>
<td>Select</td>
<td>Using the mouse, point to an icon, a button, or other item and click the left mouse button.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Convention</th>
<th>Definition or type of information</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Blue</strong></td>
<td>Identifies a cross-reference.</td>
</tr>
<tr>
<td><strong>Bold</strong></td>
<td>Identifies a selectable icon, button, menu, or tab, for example, the OK button. It also indicates the name of a field, window, dialog box, or panel.</td>
</tr>
<tr>
<td><strong>Code</strong></td>
<td>Identifies text that is displayed on the screen, or text that the user must enter.</td>
</tr>
<tr>
<td><strong>Italics</strong></td>
<td>Used to emphasize text or identifies a component of an equation or a formula.</td>
</tr>
<tr>
<td><strong>NOTE</strong></td>
<td>Alerts the user to important information.</td>
</tr>
</tbody>
</table>
Part 9 – Advanced Calibration

2 – Using Advanced Calibration parameter files

2.1 Introduction

The files calib_par_85_CTRIM.cmd and calib_par_85_tables.cmd are text files, which can be viewed by any text editor. No encryption of the calibrated parameters is used. The files can be copied to other locations and edited.

Both parameter files can be used by inserting them in DIOS with the DIOS @ command. The DIOS statement @filename inserts the contents of filename at the position of the statement. DIOS will find all files that are in the current directory, or the specified directory (if filename contains a directory path), or the directory $ISEROOT/tcad/$ISERELEASE/lib/dioslib. In Section 2.2, the rules for insertion of the parameter files are explained.

In order to understand how the Advanced Calibration works, it is useful to know the structure of the parameters files (see Section 2.3 on page 9.7).

In Section 2.4 on page 9.9, some recommendations are given as to when to use Crystal-TRIM (calib_par_85_CTRIM.cmd) and when to use tables (calib_par_85_tables.cmd) for implantations.

As an alternative to inserting the parameter files, it is possible to set the calibrated model switches and parameters directly in the DIOS input files (see Section 2.5 on page 9.10).

In Section 2.6 on page 9.19, the usage of the dose loss model with the Advanced Calibration is explained.

2.2 Inserting the parameter files

2.2.1 Preparation

In a process simulation with the pair diffusion model, before using the calibrated parameters, the following fundamental model switches must be placed somewhere at the beginning of a DIOS simulation:

```plaintext
repl(cont{newdiff=1,sidiff=off})
diff:{moddiff=pairdiffusion, segregation=on}
diff:{o2diff=diffusion}
```

The first line ensures that dopant diffusion is simulated in all materials. The second line switches on the pair diffusion model and the segregation model. The third line selects the oxidation model for which the oxidation-enhanced diffusion has been calibrated.

In addition, for MOSFET devices, the following line should be placed at the beginning of the simulation:

```plaintext
diff:{oxpo(b{stc0=0} as{stc0=0} p{stc0=0} in{stc0=0})))
```
This suppresses the dopant diffusion from polysilicon into the gate oxide. It is usually necessary, because the dose loss model used in the Advanced Calibration can lead to unrealistically high dopant penetration from polysilicon through the gate oxide to silicon. Section 2.6 on page 9.19 has a detailed discussion of the dose loss model.

### 2.2.2 Inserting the parameters

The calibrated parameters are inserted into the process simulation by the DIOS command lines:

```plaintext
@calib_par_85_CTRIM.cmd
```

or:

```plaintext
@calib_par_85_tables.cmd
```

Some parameters of the Advanced Calibration files are valid for the whole process simulation. Their values are set each time a parameter file is loaded. If all parameters were like this, it would be sufficient to insert the calibration file once at the beginning of the simulation. Unfortunately, this is not the case.

Some parameters depend on the implantation and diffusion conditions, for example, ifactor, which determines the number of excess interstitials after an implantation, depends on the implantation species, energy, and dose. In such a case, the parameter file contains a formula, such as ifactor=f(species, energy, dose). Here, species, energy, and dose are DIOS variables, which must be set to the appropriate values with the DIOS set command before inserting the parameter file.

Therefore, the correct way to use the calibration file is:

- Before each process step that requires to set process step–dependent parameters, insert the parameter file before this process step. This includes:
  - All implantation steps.
  - All annealing steps that proceed a Si or Ge preamorphization.
  - All annealing steps with oxidizing atmosphere.
  - All annealing steps in inert atmosphere, which follow an oxidation.

- Before inserting the parameter file, set the DIOS variables such as species, energy, and dose, which correspond to the following process step. They are needed to set the parameters of the physical models correctly.

- In total, the Advanced Calibration uses six DIOS variables to communicate between the DIOS input file and the parameters files: species, energy, dose, tilt, rotation, and po2 (partial oxygen pressure during annealing). Before the first insertion of an Advanced Calibration file, all six communication variables must be set, even those that are not actually used, for example, po2, in the case of an implantation. Table 9.3 on page 9.5 summarizes the definitions of these variables.

**NOTE** To change the value of a previously defined DIOS variable, set this variable to undefined in a first step and to the desired value in a second step, for example, set energy=undefined followed by set energy=1.
2.2.3 Example: 1D simulation with Advanced Calibration parameter file

This example of a DIOS input file shows how the Advanced Calibration parameter files can be used. In particular, it demonstrates how the set commands are used correctly. Typically, the Advanced Calibration files are loaded before all implantation steps and, in addition, before annealing steps in oxidizing atmosphere and annealing steps after Ge implantation.

In this example, for a correct interplay of all calibrated parameters, it is necessary to insert the parameter files before each implantation and before the final annealing step. Omitting the insertion at an implantation step affects not only the as-implanted profile, but also some of the diffusion parameters used in the subsequent annealing.

```
Title('Arsenic channel and Ge+B extension')
!
grid(xleft=0.000, xright=1.000, 
y(0.02, 0.003, 0, -0.01, -0.1,-0.2,-0.4,-1,-2,-5, -10, -50)
dy(2nm, 0.4nm, 1nm, 2nm, 10nm, 30nm,100nm,200nm, 600nm, 1,5))
repl(cont(maxtrl=1,autoada=-1))
subs(conc=1e14,elem=b,ysubs=0,orientation=100)
!
# --- fundamental model switches ----------------------------------
!
diff:(moddiff=pairdiffusion,o2diff:=diffusion,segregation=on)
repl(cont(newdiff=1,sidiff=off))
```

<table>
<thead>
<tr>
<th>Variable</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>species (main switch)</td>
<td>species=B  Set parameters for diffusion (all species) and B implantation</td>
</tr>
<tr>
<td></td>
<td>species=BF₂   Set parameters for diffusion (all species) and BF₂ implantation</td>
</tr>
<tr>
<td></td>
<td>species=As    Set parameters for diffusion (all species) and As implantation</td>
</tr>
<tr>
<td></td>
<td>species=P     Set parameters for diffusion (all species) and P implantation</td>
</tr>
<tr>
<td></td>
<td>species=In    Set parameters for diffusion (all species) and In implantation</td>
</tr>
<tr>
<td></td>
<td>species=Sb    Set parameters for diffusion (all species) and Sb implantation</td>
</tr>
<tr>
<td></td>
<td>species=Ge    Set parameters for diffusion (all species) and Ge implantation</td>
</tr>
<tr>
<td></td>
<td>species=I     Set parameters for diffusion (all species) and Si implantation</td>
</tr>
<tr>
<td>species=diff</td>
<td>Set parameters for diffusion only (all species)</td>
</tr>
<tr>
<td>species=diff_special</td>
<td>Set parameters for a diffusion step in oxidizing atmosphere or a diffusion step after Ge or Si implantation</td>
</tr>
<tr>
<td>species=default</td>
<td>Set all diffusion and implantation parameters back to DIOS default values</td>
</tr>
<tr>
<td>energy</td>
<td>Implantation energy [keV], used for implantations</td>
</tr>
<tr>
<td>dose</td>
<td>Implantation dose [cm⁻²], used for implantations</td>
</tr>
<tr>
<td>tilt</td>
<td>Implantation tilt angle, used for implantations</td>
</tr>
<tr>
<td>rotation</td>
<td>Implantation rotation angle, used for implantations</td>
</tr>
<tr>
<td>po2</td>
<td>Oxygen partial pressure [atm], used for species=diff_special</td>
</tr>
</tbody>
</table>

Table 9.3 All communication variables for calib_par_85_CTRIM.cmd and calib_par_85_tables.cmd
! --- natural oxide layer -----------------------------------------
! deposit(mat=ox, thickness=1.5nm)

! --- arsenic implantation and anneal with calibrated parameters ---
! before the first insertion of calib_par_85_tables.cmd,
! all six communication parameters must be set, even those, which are not used.
!
set species=As
set energy=100
set dose=1e13
set tilt=7
set rotation=0
set po2=0
@calib_par_85_tables.cmd
impl(element=arsenic, energy=100keV, dose=1e13, tilt=7, rotation=0)
diff(temp=(500, 1050, 1050, 500), time=(9s, 10s, 9s))

! --- Ge pre-amorphization with calibrated parameters ----------
!
set species=undefined
set species=Ge
set energy=undefined
set energy=10
set dose=undefined
set dose=2e+15
set tilt=undefined
set tilt=0
@calib_par_85_tables.cmd
impl(element=Ge, energy=10, dose=2e+15, tilt=0)

! --- B implantation with calibrated parameters ------------------
!
set species=undefined
set species=B
set energy=undefined
set energy=0.6
set dose=undefined
set dose=8e+14
@calib_par_85_tables.cmd
impl(element=B, energy=0.6, dose=8e+14, tilt=0)

! --- RTA with diffusion parameters after Ge implantation -------
!
set species=undefined
set species=diff_special
@calib_par_85_tables.cmd
diff(temp=(500, 900, 900, 800) time=(4s, 8s, 4s))

! --- Save the result
!
1D(file=result.plx format=plx factor=-1000 append=off spec(AsTotal, GeTotal, BTotal))
end
2.2.4 Returning to default parameters

All of the parameters changed in the Advanced Calibration file can be reset to their DIOS default values by using the following three lines:

```
set species=undefined
set species=default
@calib_par_85_tables.cmd
```

After switching back to default values, the accuracy of implantation, diffusion, and dose loss simulation of ultra shallow junctions is most probably reduced.

The following switches, which represent the deepest level of model selection, are not changed:

```
repl(cont(newdiff=1,sidiff=off))
diff:(o2diff=diffusion,segregation=on)
diff:(moddiff=pairdiffusion)
```

These basic selections such as moddiff=pairdiffusion are not part of the Advanced Calibration file and are usually set at the beginning of a DIOS simulation.

2.3 Structure of the parameter files

2.3.1 Overview

Both `calib_par_85_CTRIM.cmd` and `calib_par_85_tables.cmd` have the same structure and consist of three parts:

- Initialization
- General part
- Special sections depending on the DIOS variable `species`

2.3.2 Initialization

The Advanced Calibration files use some DIOS variables to track the process history. The first time, when the parameter files are inserted, these variables are initialized.

The initialization part is a block of `set` statements in an `#if`-clause:

```
#if @< $initial_advancedcalib=1 >@
#else
set initial_advancedcalib=1
set sgfac=1
set SG_B=1
set after_PAI=0
set channel=
set PAI_c10=
#endif
```

The variable `initial_advancedcalib` causes the `set` statements to be executed only the first time the parameter file is inserted.
The meaning of all process history variables is explained in Chapter 3 on page 9.21. channel and PAI_c10 are set to empty strings at the beginning.

For example, after_PAI=0 corresponds to the (initial) situation that there was no preamorphization implantation. After a Ge or Si implantation, after_PAI is set to 1. After diffusion statements, after_PAI reverts to 0. In other sections of the parameter file, after_PAI is used for setting the values of parameters that are different for simulations with and without preamorphization.

### 2.3.3 General part

The general part of the parameter files is executed each time the parameter files are inserted. Two kinds of parameters are set:

- **Diffusion parameters**, which do not depend on implantation conditions. These include, for example, diffusivities and pairing constants of dopant-interstitial and dopant-vacancy pairs. These do not include, in general, the initial activation of dopants after implantation.

- **Implantation common models and parameters**. Some parameters, for example, ifactor, can be overwritten in the following parts of the calibration file, depending on the implantation conditions. In addition, there are some ‘undefined’ entries such as dacc=undefined. By setting a parameter to undefined, the default value is used in the next implantation statement. This command is necessary if the parameter has been set to a value in a previous command.

**NOTE** The Advanced Calibration is based on the assumption that all parameters, which are not changed in the parameter files, are DIOS default parameters.

### 2.3.4 Special sections

After the general part of the parameter file, an additional section is inserted, which depends on the value of the DIOS parameter species. These sections are structured in the following way:

- **species=B, BF2, As, P, In, SB, Ge, or I**

Here, parameters are set that are related to the implantation of one of these species. These parameters are either directly related to the subsequent DIOS implantation command, for example:

```
impl:{ifactor=...}
```

or they are meant to change the diffusion after the implantation, for example:

```
diff:{acinit=...}
```

For some DIOS parameters, formulas are used, for example:

```
impl:{vfactor=0.1*$energy/(20+$energy)}
```

in the case of arsenic implantation. In such formulas, the expressions $energy, $dose, and so on are replaced by the values (or strings), which have been set before the insertion of the parameter file.
In this section, a couple of diffusion parameters are set, which are needed only for two cases: After preamorphization or for diffusion in oxidizing atmosphere. In both cases, it is recommended to insert the Advanced Calibration parameter file before the DIOS diffusion command:

```bash
#if $species=diff_special
  $PAI_cl0
diff:(siox(B{sg0=$SG_B*(0.0005+$po2)/(0.0005+2.2*$po2)\}))
  set after_PA1=undefined
  set after_PA1=0
#endif
```

$PAI_cl0 is an example for the use of a process history parameter. After initialization (see Section 2.3.2 on page 9.7), $PAI_cl0 is an empty string, and the DIOS command line $PAI_cl0 has no effect. After a Ge or Si implantation (that is, after loading the parameter file with species=Ge or species=I), $PAI_cl0 is set to a string, which is a full DIOS command line in which the value of the interstitial solid solubility is changed. As a consequence, inserting $PAI_cl0 will change this interstitial parameter if the diffusion occurs after a preamorphization implantation, reflecting the influence of preamorphization damage on interstitials.

For this choice, all models and parameters affected by the Advanced Calibration file revert to the default values (see Section 2.2.4 on page 9.7).

### 2.4 Crystal-TRIM or implantation tables?

After insertion of the file `calib_par_85_CTRIM.cmd`, the next implantation is performed with the Monte Carlo code Crystal-TRIM. After inserting `calib_par_85_tables.cmd`, the subsequent implantation will be performed by using the new ISE lookup tables. In Table 9.4, both possibilities are compared. Only the as-implanted profiles and, in some cases, the amorphization depth are affected by the choice of the parameter file, while all diffusion parameters are the same for both parameter files.

<table>
<thead>
<tr>
<th>Crystal-TRIM Implantation tables</th>
<th>Implantation tables</th>
</tr>
</thead>
<tbody>
<tr>
<td>Long CPU time (especially for high implantation energies)</td>
<td>Fast simulation of as-implanted profiles</td>
</tr>
<tr>
<td>Accurate simulations in arbitrary 2D structures</td>
<td>Limited accuracy for lateral struggling in 2D structures</td>
</tr>
<tr>
<td>Physics-based crystal damage accumulation for subsequent implantations</td>
<td>Effect of preceding implantations on ion channeling is taken into account by relatively crude models</td>
</tr>
</tbody>
</table>

The only disadvantage of using Crystal-TRIM is the CPU time needed to perform the simulation of an implantation, in particular for high implantation energy. It can be lowered by reducing the number of particles, but this will also reduce the accuracy of the Monte Carlo simulation.
The tables were generated [1] with the help of Crystal-TRIM, using the same Crystal-TRIM parameters as in calib_par_85_CTRIM.cmd. Therefore, they will usually give approximately the same as-implanted profiles as Crystal-TRIM, with the following exceptions:

- In 2D implantations, the lateral straggling is less accurate in the analytical implantation. In cases, where the lateral ion scattering is very important (for example, halo implantation into deep submicron MOSFET structures), Crystal-TRIM will give more accurate results.
- In subsequent implantations, where the first implantation reduces the channeling of ions during the latter implantations.
- In investigations of the influence of the rotation angle on the profile tail. In the implantation tables, the influence of the rotation is ignored.

For the above-mentioned cases, where the accuracy of Crystal-TRIM is superior to analytical implantation, use either calib_par_85_CTRIM.cmd or calib_par_85_tables.cmd, depending on the importance of computation speed versus accuracy.

For implantations into 1D structures (including for example, all 1D simulations or CMOS well-implantation) and implantations where the accuracy of the lateral scattering is not too important (for example, CMOS source/drain implantation), it is recommended to use the parameter file calib_par_85_tables.cmd.

It is possible to use both parameter files in the same DIOS input file. For example, in a CMOS flow, it is reasonable to perform the well and source/drain implantation with the implantation tables, and the extension implantation with Crystal-TRIM. In subsequent implantations without in-between diffusion steps, it is recommended to insert the same calibration file for each of the implantations, because the way Crystal-TRIM represents the crystal damage is ignored by analytical implantations and vice versa.

2.5 Directly inserting parameters

The calibrated parameters can be used without inserting the Advanced Calibration files. In this case, they are written directly in the process simulator input files. This approach is effective and flexible, but less convenient than inserting the complete parameter files. The parameters can be easily changed for the purpose of additional calibration.

By direct insertion, it is possible to insert only a part of the parameters, for example, only those parameters that are related to implantation, but not the diffusion parameters.

**NOTE** In DIOS, an implantation or diffusion command with a colon is not a process step, but serves to change default parameter values. For example, `impl:(dacc=0.8)` sets `dacc` to 0.8 for the subsequent implantations. To use a parameter value only for a single implantation or diffusion command, it can be written directly into the command without a colon, for example:

```
impl(element=as, energy=20keV, tilt=0, dose=1e14, dacc=0.8)
```

In order to support the direct insertion of parameters, all parameters and the corresponding DIOS syntax are summarized in the following tables. An example is provided in Section 2.5.1 on page 9.17. The meaning of the parameters is further explained in Chapter 3 on page 9.21.
### Table 9.5  
Set of calibrated parameters for dopant distribution after implantation (with Crystal-TRIM)

<table>
<thead>
<tr>
<th>Implantation species</th>
<th>Parameter</th>
<th>Value</th>
<th>DIOS command</th>
<th>Effect</th>
</tr>
</thead>
<tbody>
<tr>
<td>All</td>
<td>function</td>
<td>newCrystal Trim</td>
<td>impl:(function=newCrystalTrim)</td>
<td>MC code for implantation is used.</td>
</tr>
<tr>
<td></td>
<td>particles</td>
<td>8000</td>
<td>impl:(particles=8000)</td>
<td>Statistics of MC simulation</td>
</tr>
<tr>
<td></td>
<td>polyOri</td>
<td>0</td>
<td>impl:(polyOri=0)</td>
<td>Poly-Si is treated as amorphous Si for implantation</td>
</tr>
<tr>
<td>B</td>
<td>cex1</td>
<td>cex1=f(E)(^1)</td>
<td>impl:(cex1=value)</td>
<td>Electronic stopping &lt;110&gt;</td>
</tr>
<tr>
<td></td>
<td>cex2</td>
<td>cex2=f(E)</td>
<td>impl:(cex2=value)</td>
<td>Electronic stopping &lt;100&gt;(^2)</td>
</tr>
<tr>
<td></td>
<td>dacc</td>
<td>0.1</td>
<td>impl:(dacc=0.1)</td>
<td>Damage accumulation</td>
</tr>
<tr>
<td></td>
<td>dcrit</td>
<td>1</td>
<td>impl:(dcrit=1)</td>
<td>Threshold for amorphization</td>
</tr>
<tr>
<td>BF(_2)</td>
<td>cex1</td>
<td>cex1=f(E)</td>
<td>impl:(cex1=value)</td>
<td>Electronic stopping &lt;110&gt;</td>
</tr>
<tr>
<td></td>
<td>dacc</td>
<td>0.15</td>
<td>impl:(dacc=0.15)</td>
<td>Damage accumulation</td>
</tr>
<tr>
<td></td>
<td>dcrit</td>
<td>0.05</td>
<td>impl:(dcrit=0.05)</td>
<td>Threshold for amorphization</td>
</tr>
<tr>
<td>As</td>
<td>dacc</td>
<td>dacc=f(E)</td>
<td>impl:(dacc=value)</td>
<td>Damage accumulation</td>
</tr>
<tr>
<td>In</td>
<td>dacc</td>
<td>0.7</td>
<td>impl:(dacc=0.7)</td>
<td>Damage accumulation</td>
</tr>
<tr>
<td></td>
<td>amav</td>
<td>1.04</td>
<td>impl:(amav=1.04)</td>
<td>Range in amorphous regions</td>
</tr>
<tr>
<td></td>
<td>amdev</td>
<td>0</td>
<td>impl:(amdev=0)</td>
<td>Standard deviation of range in amorphous regions</td>
</tr>
<tr>
<td>Sb</td>
<td>dacc</td>
<td>1.0</td>
<td>impl:(dacc=1.0)</td>
<td>Damage accumulation</td>
</tr>
<tr>
<td></td>
<td>dcrit</td>
<td>0.2</td>
<td>impl:(dcrit=0.2)</td>
<td>Threshold for amorphization</td>
</tr>
<tr>
<td></td>
<td>amav</td>
<td>0.93</td>
<td>impl:(amav=0.93)</td>
<td>Range in amorphous regions</td>
</tr>
<tr>
<td></td>
<td>amdev</td>
<td>amdev=f(E)</td>
<td>impl:(amdev=value)</td>
<td>Standard deviation of range in amorphous regions</td>
</tr>
</tbody>
</table>

1. \(cex1=f(E)\) means that the value depends on the implantation energy. The formula can be looked up in the parameter file `calib_par_85_CTRIM.cmd`.
2. More precisely: All directions other than <110>.

9.11
### Table 9.6 Set of calibrated parameters for dopant distribution after implantation (with analytical tables) (all table names are listed in Chapter 6 on page 9.59)

<table>
<thead>
<tr>
<th>Implantation species</th>
<th>Parameter</th>
<th>Value</th>
<th>DIOS command</th>
<th>Effect</th>
</tr>
</thead>
<tbody>
<tr>
<td>All</td>
<td>totaldose</td>
<td>dose</td>
<td><code>impl:(si(totaldose=value))</code></td>
<td>To be used together with channelingdose; not required for a single implantation</td>
</tr>
<tr>
<td></td>
<td>channeling dose</td>
<td>channeling dose=value</td>
<td><code>impl:(si(channelingdose=value))</code></td>
<td>Dose of channeling ions for dual Pearson tables; not required for a single implantation. After preamorphization, channelingdose should be set to a low value.</td>
</tr>
<tr>
<td>B</td>
<td>table</td>
<td>table=name</td>
<td><code>impl:(table=name)</code></td>
<td>Implantation table</td>
</tr>
<tr>
<td>BF₂</td>
<td>table</td>
<td>table=name</td>
<td><code>impl:(table=name)</code></td>
<td>Implantation table</td>
</tr>
<tr>
<td>As</td>
<td>table</td>
<td>table=name</td>
<td><code>impl:(table=name)</code></td>
<td>Implantation table</td>
</tr>
<tr>
<td>P</td>
<td>table</td>
<td>table=name</td>
<td><code>impl:(table=name)</code></td>
<td>Implantation table</td>
</tr>
<tr>
<td>In</td>
<td>table</td>
<td>table=name</td>
<td><code>impl:(table=name)</code></td>
<td>Implantation table</td>
</tr>
<tr>
<td>Sb</td>
<td>table</td>
<td>table=name</td>
<td><code>impl:(table=name)</code></td>
<td>Implantation table</td>
</tr>
<tr>
<td>Ge</td>
<td>table</td>
<td>table=name</td>
<td><code>impl:(table=name)</code></td>
<td>Implantation table</td>
</tr>
</tbody>
</table>

### Table 9.7 Set of calibrated parameters for initial conditions after implantation

<table>
<thead>
<tr>
<th>Implantation species</th>
<th>Parameter</th>
<th>Value</th>
<th>DIOS command</th>
<th>Effect</th>
</tr>
</thead>
<tbody>
<tr>
<td>All</td>
<td>damage</td>
<td>+1</td>
<td><code>impl:(damage=+1)</code></td>
<td>damage+x model for interstitials and vacancies</td>
</tr>
<tr>
<td></td>
<td>amorphization</td>
<td>mcdamage</td>
<td><code>impl:(amorphization=value)</code></td>
<td>Amorphization model</td>
</tr>
<tr>
<td></td>
<td></td>
<td>hobler</td>
<td><code>impl:(amorphization=value)</code></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>+1</td>
<td><code>impl:(amorphization=value)</code></td>
<td></td>
</tr>
<tr>
<td></td>
<td>ifactor</td>
<td>ifactor=f(E, dose)</td>
<td><code>impl:(ifactor=value)</code></td>
<td>Initial amount of interstitials</td>
</tr>
<tr>
<td></td>
<td>vfactor</td>
<td>0</td>
<td><code>impl:(vfactor=0)</code></td>
<td>Initial amount of vacancies</td>
</tr>
<tr>
<td></td>
<td>acinit</td>
<td>acinit=f(E, dose)</td>
<td><code>impl:(acinit=value)</code></td>
<td>Initial dopant activation in crystalline region</td>
</tr>
<tr>
<td></td>
<td>aminit</td>
<td>3.5e20</td>
<td><code>impl:(acinit=value)</code></td>
<td>Initial B activation in recrystallized regions</td>
</tr>
</tbody>
</table>

9.12
### Table 9.7  Set of calibrated parameters for initial conditions after implantation

<table>
<thead>
<tr>
<th>Implantation species</th>
<th>Parameter</th>
<th>Value</th>
<th>DIOS command</th>
<th>Effect</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>BF$_2$</strong></td>
<td>ifactor</td>
<td>$f(E)$</td>
<td>impl:(ifactor=value)</td>
<td>Initial amount of interstitials</td>
</tr>
<tr>
<td></td>
<td>vfactor</td>
<td>0</td>
<td>impl:(vfactor=0)</td>
<td>Initial amount of vacancies</td>
</tr>
<tr>
<td></td>
<td>acinit</td>
<td>3e17</td>
<td>diff:(acinit=3e17)</td>
<td>Initial dopant activation in crystalline region</td>
</tr>
<tr>
<td></td>
<td>aminit</td>
<td>$3.5e20$ usually $f(E)$ after pre-amorphization</td>
<td>diff:(si(b(aminit=value)))</td>
<td>Initial B activation in recrystallized regions</td>
</tr>
<tr>
<td><strong>As</strong></td>
<td>ifactor</td>
<td>$f(E, \text{dose})$</td>
<td>impl:(ifactor=value)</td>
<td>Initial amount of interstitials</td>
</tr>
<tr>
<td></td>
<td>vfactor</td>
<td>$f(E)$</td>
<td>impl:(vfactor=value)</td>
<td>Initial amount of vacancies</td>
</tr>
<tr>
<td></td>
<td>acinit</td>
<td>$f(\text{dose})$</td>
<td>diff:(acinit=value)</td>
<td>Initial As activation</td>
</tr>
<tr>
<td></td>
<td>aminit</td>
<td>$2.5e20$</td>
<td>diff:(si(as(aminit=2.5e20)))</td>
<td>Initial As activation in recrystallized regions</td>
</tr>
<tr>
<td><strong>In</strong></td>
<td>ifactor</td>
<td>1</td>
<td>impl:(ifactor=value)</td>
<td>Initial amount of interstitials</td>
</tr>
<tr>
<td></td>
<td>vfactor</td>
<td>0</td>
<td>impl:(vfactor=value)</td>
<td>Initial amount of vacancies</td>
</tr>
<tr>
<td></td>
<td>afactor</td>
<td>1200</td>
<td>impl:(afactor=1200)</td>
<td>Scaling of amorphization (for amorphization=+1)</td>
</tr>
<tr>
<td></td>
<td>acinit</td>
<td>$2e18$</td>
<td>diff:(acinit=2e18)</td>
<td>Initial In activation</td>
</tr>
<tr>
<td><strong>Sb</strong></td>
<td>ifactor</td>
<td>1</td>
<td>impl:(ifactor=value)</td>
<td>Initial amount of interstitials</td>
</tr>
<tr>
<td></td>
<td>vfactor</td>
<td>0</td>
<td>impl:(vfactor=value)</td>
<td>Initial amount of vacancies</td>
</tr>
<tr>
<td><strong>P</strong></td>
<td>ifactor</td>
<td>1</td>
<td>impl:(ifactor=value)</td>
<td>Initial amount of interstitials</td>
</tr>
<tr>
<td></td>
<td>vfactor</td>
<td>0</td>
<td>impl:(vfactor=value)</td>
<td>Initial amount of vacancies</td>
</tr>
<tr>
<td><strong>Ge</strong></td>
<td>ifactor</td>
<td>1</td>
<td>impl:(ifactor=value)</td>
<td>Initial amount of interstitials</td>
</tr>
<tr>
<td></td>
<td>vfactor</td>
<td>0</td>
<td>impl:(vfactor=value)</td>
<td>Initial amount of vacancies</td>
</tr>
<tr>
<td></td>
<td>afactor</td>
<td>$f(E)$</td>
<td>impl:(afactor=value)</td>
<td>Scaling of amorphization</td>
</tr>
<tr>
<td></td>
<td>(used for analytical implantation)</td>
<td>afactor=$f(E)$</td>
<td>impl:(afactor=value)</td>
<td>Scaling of amorphization</td>
</tr>
<tr>
<td></td>
<td>threshold</td>
<td>$f(E)$</td>
<td>impl:(threshold=value)</td>
<td>Amorphization threshold</td>
</tr>
<tr>
<td></td>
<td>(used for MC implantation)</td>
<td>threshold=$f(E)$</td>
<td>impl:(threshold=value)</td>
<td>Amorphization threshold</td>
</tr>
<tr>
<td><strong>I</strong></td>
<td>ifactor</td>
<td>0</td>
<td>impl:(ifactor=0)</td>
<td>Excess interstitials</td>
</tr>
<tr>
<td></td>
<td>vfactor</td>
<td>0</td>
<td>impl:(vfactor=0)</td>
<td>Initial amount of vacancies</td>
</tr>
</tbody>
</table>
Table 9.7  Set of calibrated parameters for initial conditions after implantation

<table>
<thead>
<tr>
<th>Implantation species</th>
<th>Parameter</th>
<th>Value</th>
<th>DIOS command</th>
<th>Effect</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>afactor</td>
<td>afactor=f(E)</td>
<td>impl:(afactor=value)</td>
<td>Scaling of amorphization</td>
</tr>
<tr>
<td></td>
<td>threshold</td>
<td>threshold=f(E)</td>
<td>impl:(threshold=value)</td>
<td>Amorphization threshold</td>
</tr>
</tbody>
</table>

Table 9.8  Parameters changed from default for diffusivities, pairing constants, and point defect boundary conditions in silicon

<table>
<thead>
<tr>
<th>Implantation species</th>
<th>Parameter</th>
<th>Value</th>
<th>DIOS command</th>
<th>Effect</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>poxo</td>
<td>poxo=2.7e-4</td>
<td>diff:(si(i(pox=2.7e-4, poxo=-2)))</td>
<td>Boundary conditions for oxidation-enhanced diffusion</td>
</tr>
<tr>
<td></td>
<td>potox</td>
<td>potox=-2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>V</td>
<td>BC_typ</td>
<td>HomNeumann</td>
<td>diff:(si(o(v(BC_typ=HomNeumann)))) diff:(si(i(v(BC_typ=HomNeumann))))</td>
<td>No vacancy flux into or from silicon surfaces</td>
</tr>
<tr>
<td>B</td>
<td>dipB</td>
<td>1.25</td>
<td>diff:(si(b(dip=1.25)))</td>
<td>Diffusivity of (B – I+) pairs (Arrhenius prefactor)</td>
</tr>
<tr>
<td></td>
<td>di00, di0w</td>
<td>di00=0.033, di0w=3.26</td>
<td>diff:(si(b(di00=0.033, di0w=3.26)))</td>
<td>Diffusivity of (B – I0) pairs (Arrhenius constant)</td>
</tr>
<tr>
<td></td>
<td>q(ge)</td>
<td>125</td>
<td>diff:(si(b(q(ge=125))))</td>
<td>Coupling factor between B pair diffusivity and Ge concentration</td>
</tr>
<tr>
<td>As</td>
<td>dimm0, dimm</td>
<td>dimm0=800, dimm=4.75</td>
<td>diff:(si(a(dimm0=800, dimm=4.75)))</td>
<td>Diffusivity of (As – I–) pairs (Arrhenius constant)</td>
</tr>
<tr>
<td></td>
<td>dim0</td>
<td>12</td>
<td>diff:(si(a(dim=12)))</td>
<td>Diffusivity of (As – I+ ) pairs (Arrhenius prefactor)</td>
</tr>
<tr>
<td></td>
<td>pi0mm, pimm</td>
<td>pi0mm=3.6e-30, pimm=1.75</td>
<td>diff:(si(a(pi0mm=3.6e-30, pimm=1.75)))</td>
<td>Pairing constant of (As – I–) pairs (Arrhenius constant)</td>
</tr>
<tr>
<td></td>
<td>dvm0</td>
<td>3</td>
<td>diff:(si(a(dvm=3)))</td>
<td>Diffusivity of (As – V+) pairs (Arrhenius prefactor)</td>
</tr>
<tr>
<td></td>
<td>dvmm0</td>
<td>0.02</td>
<td>diff:(si(a(dvmm=0.02)))</td>
<td>Diffusivity of (As – V0) pairs (Arrhenius prefactor)</td>
</tr>
<tr>
<td></td>
<td>pv0m</td>
<td>2e-26</td>
<td>diff:(si(a(pv=2e-26)))</td>
<td>Pairing constant of (As – V+) pairs (Arrhenius prefactor)</td>
</tr>
<tr>
<td>As</td>
<td>pv00</td>
<td>2e-26</td>
<td>diff:(si(a(pv0=2e-26)))</td>
<td>Pairing constant of (As – V0) pairs (Arrhenius prefactor)</td>
</tr>
</tbody>
</table>
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Table 9.8  Parameters changed from default for diffusivities, pairing constants, and point defect boundary conditions in silicon

<table>
<thead>
<tr>
<th>Implantation species</th>
<th>Parameter</th>
<th>Value</th>
<th>DIOS command</th>
<th>Effect</th>
</tr>
</thead>
<tbody>
<tr>
<td>P</td>
<td>pi00</td>
<td>1.8e-20</td>
<td>diff:(si(p(pi00=1.8e-20)))</td>
<td>Pairing constant of ((P^+ I^0)) pairs (Arrhenius prefactor)</td>
</tr>
<tr>
<td></td>
<td>dim0, dimw</td>
<td>dim0=0.0026, dimw=3.05</td>
<td>diff:(si(p(dim0=0.0026, dimw=3.05)))</td>
<td>Diffusivity of ((As^+ I^-)) pairs (Arrhenius constant)</td>
</tr>
<tr>
<td></td>
<td>di00</td>
<td>0.7</td>
<td>diff:(si(as(di00=0.7)))</td>
<td>Diffusivity of ((As^+ I^-)) pairs (Arrhenius prefactor)</td>
</tr>
<tr>
<td></td>
<td>q(as)</td>
<td>500</td>
<td>diff:(si(p(q(as=500))))</td>
<td>Coupling factor between P pair diffusivity and As concentration</td>
</tr>
<tr>
<td>In</td>
<td>pi00</td>
<td>3.5e-27</td>
<td>diff:(si(in(pi00=3.5e-27)))</td>
<td>Pairing constant of ((In^- I^0)) pairs (Arrhenius prefactor)</td>
</tr>
<tr>
<td></td>
<td>di00, di0w</td>
<td>di00=1.568, di0w=3.5645</td>
<td>diff:(si(b(di00=1.568, di0w=3.5645)))</td>
<td>Diffusivity of ((In^- I^-)) pairs (Arrhenius constant)</td>
</tr>
<tr>
<td></td>
<td>dip0</td>
<td>0</td>
<td>diff:(si(b(dip0=0)))</td>
<td>Diffusivity of ((In^- I^-)) pairs</td>
</tr>
<tr>
<td></td>
<td>q(n)(^1)</td>
<td>1.5e4</td>
<td>diff:(si(in(q(n=1.5e4))))</td>
<td>Coupling factor between In pair diffusivity and N concentration</td>
</tr>
<tr>
<td>Sb</td>
<td>dv00</td>
<td>0.2568</td>
<td>diff:(si(sb(dv00=0.2568)))</td>
<td>Diffusivity of ((Sb^+ V^0)) pairs (Arrhenius prefactor)</td>
</tr>
</tbody>
</table>

\(^1\) The meaning of this parameter is further explained in Section 3.8 on page 9.30.

Table 9.9  Calibrated parameter for interstitial release (related to TED)

<table>
<thead>
<tr>
<th>Implantation species</th>
<th>Parameter</th>
<th>Value</th>
<th>DIOS command</th>
<th>Effect</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>c10</td>
<td>Depends strongly on implantation conditions</td>
<td>diff:(si(i(c10=value)))</td>
<td>Interstitial solid solubility. A low value results in a slow dissolution of I-clusters.</td>
</tr>
</tbody>
</table>

Table 9.10  Calibrated parameters for dopant clustering

<table>
<thead>
<tr>
<th>Implantation species</th>
<th>Parameter</th>
<th>Value</th>
<th>DIOS command</th>
<th>Effect</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>modclust</td>
<td>transient</td>
<td>diff:(si(b(modclust=transient)))</td>
<td>Nonequilibrium clustering model for B</td>
</tr>
<tr>
<td></td>
<td>c10</td>
<td>c10=2e22</td>
<td>diff:(si(b(c10=2e22)))</td>
<td>Solid solubility of B in Si (Arrhenius prefactor)</td>
</tr>
</tbody>
</table>
Table 9.11 lists the calibrated parameters for dose loss modeling. It is assumed that the silicon is covered by oxide. The dose loss model used is discussed in detail in Section 2.6 on page 9.19 and Chapter 3 on page 9.21. The table entries for Sb are for segregation into oxide.

Table 9.11  Calibrated parameters for dose loss modeling at the Si–SiO₂ interface

<table>
<thead>
<tr>
<th>Implantation species</th>
<th>Parameter</th>
<th>Value</th>
<th>DIOS command</th>
<th>Effect</th>
</tr>
</thead>
<tbody>
<tr>
<td>B, BF₂</td>
<td>di0, diw</td>
<td>di0=0.01, diw=3.6</td>
<td>diff:(ox(b{di0=0.01, diw=3.6}))</td>
<td>Increased diffusivity in SiO₂ to reduce mesh noise.  (Arrhenius constant)</td>
</tr>
<tr>
<td></td>
<td>stc0, stcw</td>
<td>stc0=1e27, stcw=6</td>
<td>diff:(siox(b{stc0=1e27, stcw=6}))</td>
<td>Flux parameter for B segregation. At high temperatures, the dose loss is limited by the segregation coefficient.</td>
</tr>
<tr>
<td></td>
<td>sg0, sgw</td>
<td>sg0 depends on implantation condition and process history. sgw=0</td>
<td>diff:(siox(b{sg0= value, sgw=0}))</td>
<td>Segregation coefficient between Si and SiO₂. Fixes the amount of dose loss.  (Arrhenius constant)</td>
</tr>
</tbody>
</table>
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Table 9.11  Calibrated parameters for dose loss modeling at the Si–SiO₂ interface

<table>
<thead>
<tr>
<th>Implantation species</th>
<th>Parameter</th>
<th>Value</th>
<th>DIOS command</th>
<th>Effect</th>
</tr>
</thead>
<tbody>
<tr>
<td>As</td>
<td>d₁₀, d₁₅</td>
<td>di₀=0.01, di₁₅=3.6</td>
<td>diff: (ox(as(di₀=0.01, di₁₅=3.6)))</td>
<td>Increased diffusivity in SiO₂ to reduce mesh noise</td>
</tr>
<tr>
<td></td>
<td>stc₀</td>
<td>1e14</td>
<td>diff: (siox(as(stc₀=1e14)))</td>
<td>High flux parameter. --&gt; Dose loss is limited by the segregation constant.</td>
</tr>
<tr>
<td></td>
<td>sg₀, sg₁₅</td>
<td>sg₀ depends on implantation condition, sg₁₅=0</td>
<td>diff: (siox(as(sg₀= value, sg₁₅=0)))</td>
<td>Segregation coefficient between Si and SiO₂. Fixes the amount of dose loss.</td>
</tr>
<tr>
<td>P</td>
<td>d₁₀, d₁₅</td>
<td>di₀=0.01, di₁₅=3.6</td>
<td>diff: (ox(p(di₀=0.01, di₁₅=3.6)))</td>
<td>Increased diffusivity in SiO₂ to reduce mesh noise</td>
</tr>
<tr>
<td></td>
<td>stc₀</td>
<td>1e14</td>
<td>diff: (siox(p(stc₀=1e14)))</td>
<td>High flux parameter. --&gt; Dose loss is limited by the segregation constant.</td>
</tr>
<tr>
<td></td>
<td>sg₀, sg₁₅</td>
<td>sg₀=50, sg₁₅=0</td>
<td>diff: (siox(p(sg₀=50, sg₁₅=0)))</td>
<td>Segregation coefficient between Si and SiO₂.</td>
</tr>
<tr>
<td>In</td>
<td>stc₀, stc₁₅</td>
<td>stc₀=1e4, stc₁₅=0</td>
<td>diff: (siox(in(stc₀=1e4, stc₁₅=0)))</td>
<td>For a very high flux parameter and segregation coefficient, the In dose loss is diffusion limited.</td>
</tr>
<tr>
<td></td>
<td>sg₀, sg₁₅</td>
<td>sg₀=1e5, sg₁₅=0</td>
<td>diff: (siox(in(sg₀=1e5, sg₁₅=0)))</td>
<td>Segregation coefficient between Si and SiO₂.</td>
</tr>
<tr>
<td>Sb</td>
<td>d₁₀, d₁₅</td>
<td>di₀=6.4, di₁₅=4.58</td>
<td>diff: (ox(sb(di₀=6.4, di₁₅=4.58)))</td>
<td>Diffusivity of Sb in oxide</td>
</tr>
<tr>
<td></td>
<td>sg₀</td>
<td>2</td>
<td>diff: (siox(sb(sg₀=2)))</td>
<td>Segregation coefficient between Si and oxide</td>
</tr>
<tr>
<td></td>
<td>stc₀ at SiO₂/Gas interface</td>
<td>5e4</td>
<td>diff: (oxgas(sb(stc₀=5e4)))</td>
<td>Flux parameter for the Sb out-diffusion from oxide to gas (Arrhenius prefactor)</td>
</tr>
</tbody>
</table>

2.5.1  Example for direct use of Advanced Calibration parameters

In this section, a simple example is presented that shows how the parameters can be used by direct entries into a DIOS input file. A boron drain–extension implantation is examined followed by an activation step, which is described by the following two DIOS commands:

impl (elem=b, energy=0.5, dose=5e14, tilt=0)
diff (temperature=(500, 900, 900) time=(8s, 10s))

First, the models necessary for the simulation are set:

repl (cont (newdiff=1, sidiff=off))
diff (o2diff := diffusion, segregation=on)
diff (moddiff = pairdiffusion)
Then, the global diffusion parameters are fixed; these parameters are valid for all process steps:

```plaintext
diff:(si(b(modclust=transient, c10=2e22
dip0=1.25,
d10=0.033, d10w=3.26))
ox(b(d10=0.01, d1w=3.6))
siox(b(stc0=1e27, stcw=6, sgw=0)))
```

For the B implantation, the appropriate Advanced Calibration parameters listed in Table 9.6 on page 9.12 and Table 9.7 on page 9.12 are written directly into the implantation command. For the appropriate value of \( ifactor \), the formula \( ifactor = f(energy, dose) \), which is found in the Advanced Calibration files in the section for B implantation, is evaluated:

```plaintext
impl(elem=b,energy=0.5,dose=5e14,tilt=0,
table="B_16e13-8e15.tab", damage=+1, vfactor=0,
ifactor=0.137, amorphization=hobler)
```

Alternatively, two set commands and the general formula for \( ifactor \) can be used:

```plaintext
set energy=0.5
set dose=5e14
impl(elem=b,energy=0.5,dose=5e14,tilt=0,
table="B_16e13-8e15.tab", damage=+1, vfactor=0,
ifactor=$energy/(energy+0.8)*(2e15+$dose)/(2e15+10*$dose)
*1e17/(1e17+$energy*$dose)
amorphization=mcdamage)
```

The remaining initial conditions for diffusion, which are not already contained in the above implantation statement, are defined by setting the diffusion parameters from Table 9.7 on page 9.12, Table 9.9 on page 9.15, and Table 9.11 on page 9.16. For some parameters, the table entries are only ‘depend on implantation conditions.’ These must be looked up in the section on B implantation in the Advanced Calibration files. There, one finds:

```plaintext
diff:(siox(b(sg0=60*$sgfac*(energy+1.1)/(energy+0.3)))
diff:(si(b(aminit=3.5e20)))
diff:(acinit=3e17+$dose/5e14*(1.5e18-2.4e17*$energy))
```

The process history parameter \( sgfac \) is 1 by default and is only changed by Si implantation. With \( energy=0.5 \) and \( dose=5e14 \), the formulas give the following statements for the initial conditions for diffusion:

```plaintext
diff:(siox(b(sg0=112.5)))
diff:(si(b(aminit=3.5e20)))
diff:(acinit=1.6e18)
```

Now, the activation step can follow:

```plaintext
diff(temperature=(500,900,900) time=(8s, 10s))
```

This example illustrates that it is less convenient to insert all parameters directly ‘by hand.’ In general, inserting the complete parameter file is easier and, therefore, more reliable.
2.6 Dose loss modeling

2.6.1 Model

In Advanced Calibration, the dose loss of B, As, P, and In is simulated by dopant segregation into oxide. This is a major difference to earlier versions of the Advanced Calibration, in which a thin dose loss layer of Ce was used.

Figure 9.1 Dose loss into SiO$_2$. Red line shows a simulated boron profile after 1 keV B implantation and spike annealing. Interface between Si and a 1.5 nm oxide layer is situated at depth = 0 nm. During annealing, a part of the boron has moved into the oxide layer.

In Figure 9.1, the principle of the dose loss model is illustrated. At the interface Si–SiO$_2$, the ratio of dopant concentration in silicon and oxide is governed by the segregation coefficient ($s_{g0}, s_{gw}$) and the flux parameter ($stc_0, stcw$). In the calculations for Figure 9.1, a high segregation coefficient was used. As a consequence, the dopant concentration at the oxide side of the interface is very high, and a part of the dose is ‘lost’ for carrier transport in silicon.

2.6.2 Dopant diffusivity and mesh in oxide

Inside the oxide, the diffusivity of B, As, and P is increased with respect to the default values, but still rather low. Thus, there is a very steep dopant gradient at the oxide side of the interface. From the physics point of view, this is quite reasonable. A considerable amount of dopants can be built into a few monolayers around the Si–SiO$_2$ interface. Such behavior has been measured for arsenic [2] and can also be the case for other dopants.

From the numerics viewpoint, the steep gradient causes a problem. A large fraction of the dopants in the oxide is ascribed to a single mesh point. This can lead to an overestimation of the dose loss due to numerical errors. It is necessary to have a very fine mesh at the interface in order to keep such numerical errors very small. Typically, at the oxide side of the Si–SiO$_2$ interface, the mesh point spacing should be a few angstrom only.

With the default diffusivities of B, As, and P in oxide, this numerical aspect would require even finer meshes, leading to difficulties in 2D simulations. That is the only reason why the Advanced Calibration uses increased diffusivities of B, As, and P in oxide with respect to the well-established default values.

The increased diffusivities in oxide are still much lower than dopant diffusivities in silicon. This prevents undesired artifacts, for example, a significant dopant diffusion in oxide spacer regions. Still, there may be rare
cases where the simulation result is very sensitive to dopant diffusivity in oxide. In such cases, the DIOS default values should be used for dopant diffusivity in oxide. This can be achieved by editing the parameter files.

2.6.3 Dopant penetration through a thin oxide

Using segregation into SiO₂ for the dose loss modeling creates a problem for the simulation of MOSFETs. It can happen that dopants enter the gate oxide from the poly-Si side, diffuse through the gate oxide, and exit at the silicon side (dopant penetration).

With the dose loss model used in Advanced Calibration, there can be a huge overestimation of dopant penetration through the gate oxide. It is important to avoid this. One possible way to do this is to suppress completely the dopant flux from polysilicon to silicon. The corresponding DIOS command is:

```
diff:cxpc(b(stc0=0) as(stc0=0) p(stc0=0) in(stc0=0))
```

An alternative is to replace a part of the gate oxide by another material, for example nitride, in the simulation. Then, the dopant diffusivity in nitride can be used to adjust the dopant penetration through the gate oxide.

2.6.4 Dose loss to other materials than oxide

Only dopant dose loss into SiO₂ has been calibrated so far. If silicon is covered by some other material, for example nitride, the default values for segregation are used, which usually do not give a large dose loss.

**NOTE** By placing different materials onto the Si surface, one can, if necessary, adjust different parameters for dose loss modeling on different regions of the device.

2.6.5 Outlook: Three-phase segregation model

Starting with ISE TCAD Release 8.5, a three-phase segregation model is available in DIOS, which can be used for dose loss modeling. In this model, dopants can be trapped and released at the interface of boundaries. In comparison with the standard segregation model used in the Advanced Calibration, it is more flexible and does not require any ultrafine meshes at the interfaces. However, as it has not been calibrated yet to state-of-the-art deep submicron profiles, the three-phase segregation model is not used in the Advanced Calibration.
3.1 Introduction

In this section, the parameters of the Advanced Calibration files are explained. The files contain all parameters that have been calibrated or modified from the DIOS default values in order to obtain a reasonable agreement with more than 1000 SIMS profiles. All parameters are presented in the syntax of the DIOS input language.

The most important process steps for the final dopant distribution are implantation steps and high-temperature (diffusion) steps. The latter include furnace anneals, RTA, spike anneals, and oxidations. Consequently, the modeling parameters can be separated into three types:

- Parameters for the distribution of dopants after implantation
- Parameters for the initial conditions of a diffusion after implantation (for example, implantation damage and initial dopant activation)
- Parameters for diffusion (for example, diffusivities and boundary conditions)

The parameters of the Advanced Calibration files are explained according to this scheme.

The parameters for boron (B) implantation and B-interstitial diffusion are explained in detail, after which the parameters for BF$_2$, arsenic (As) (and vacancies), indium (In), and antimony (Sb) are explained with a focus on the main differences to the B case.

A complete list of all parameters affected in the Advanced Calibration can be found in the tables of Section 2.5 on page 9.10. Additional information on the calibration methodology and the influence of the parameters is provided in Chapter 4 on page 9.37.

3.2 Boron implantation parameters (Crystal-TRIM)

First, the parameters that are used for modeling the implantation are discussed. In the Advanced Calibration file `calib_par_85_CTRIM.cmd`, the relevant implantation entries are:

```plaintext
impl:(damage=1, fitasimplanteddose=off,  
function=newCrystalTRIM, polyOri=0)
impl:(vfactor=0, amorphization=mcDamage, particles=8000)
impl:(ifactor=$energy/($energy+0.8)*(2e15+$dose)/(2e15+10*$dose)  
*1e17/(1e17+$energy*$dose))
#if $energy > 10.0
impl:(particles=3000)
#endif
#if $energy < 2.0001
impl:(cex1 = 1.0+3.0/(4.5*$energy+1.0)+30.0/(4.5*$energy+1.0)**4,  
cex2 = 1.6*($energy**-0.06)
 dacc=0.1, dcrit=1)
#endif
```
### 3.2.1 Meaning of parameter=undefined

In addition, there are some ‘undefined’ entries such as $dacc=undefined$. By setting a parameter to undefined, the default value is used in the next implantation statement. This command is necessary if the parameter has been set to a different value in a previous command.

Some other parameters are set to default values, for example, $afactor=1$ or $dmodel=6$. Again, this is necessary if the parameter has been set to an inappropriate value in a previous command.

### 3.2.2 As-implanted dopant profile

The parameters $function=newCrystalTrim$, $particles$, $cex1$, $cex2$, $dacc$, and $dcrit$ govern the calculation of the as-implanted profile for Monte Carlo implantations. $fitasimplanteddose$ governs a numerical correction for the as-implanted profile.

- The option $function=newCrystalTrim$ switches on the Monte Carlo model Crystal-TRIM in DIOS, which is more accurate but slower than analytical implantation. As an alternative for applications where the CPU time is important, implantation lookup tables, which are based on calibrated Monte Carlo simulations, can be used (see Section 2.4 on page 9.9 for a comparison). The difference with respect to $function=OldCrystalTrim$ is that the parameters $amav$ and $amdev$ (calibrated for In and Sb) are used in amorphous regions always.

- The switch $polyOri=0$ has the effect that poly-Si is treated as amorphous during implantation. The alternative, $polyOri=110$, usually leads to an overestimation of dopant channeling in poly-Si.

- $particles=8000$ fixes the number of incident Monte Carlo particles per simulation column. The value 8000 is high and leads to a slow simulation and very low statistical error. For most practical purposes, a value of 3000 is sufficient. As the simulation time for Monte Carlo implantation increases with the particle energy, $particles$ is reduced to the value 3000 for energies higher than 10 keV.

- $cex1$ and $cex2$ are used for the calculation of electronic stopping in channeling directions [3] and influence mainly the tail region of the profiles. A high value of $cex1$ increases the channeling in the $<110>$ crystal direction. A high value of $cex2$ increases the channeling in all other channeling directions, including the $<100>$ direction.

- $dacc$ scales the damage accumulation during implantation [4]. It should have a value between 0 and 1. A high value of $dacc$ corresponds to a large damage produced per deposited energy and reduces the channeling for medium and high dose implantations.

- $dcrit$ scales the amorphization threshold during implantation. It should have a value between 0 and 1. If the crystal damage exceeds a certain value, DIOS treats this region as amorphous during the implantation. The combination of $dacc=0.1$ and $dcrit=1$ suppresses amorphization for B implantation with doses less than $10^{15}$ cm$^{-2}$.

- $fitasimplanteddose$ is a switch for a numerical correction. After implantation, the as-implanted dose is integrated. On coarse meshes, this dose may deviate from the expected dose due to numerical errors. With $fitasimplanteddose=on$, the as-implanted profile is rescaled in order to match exactly the specified dose. With $fitasimplanteddose=off$, no such re-scaling is performed. The reason for switching off the re-scaling is that, in 2D simulation, the mesh is usually fine in the important device regions and coarse in the less important regions. A constant re-scaling of the dose in the whole device can transport a numerical error from the regions with coarse mesh to regions with fine mesh.
NOTE  The as-implanted profiles are not very accurate for B energies higher than 100 keV. Typically, the simulated profiles are slightly deeper than SIMS data and show more channeling. Often, better results are obtained by increasing \( d_{acc} \) or the parameter \( \text{impl}:(\lambda) \). Section 4.3 on page 9.38 sets out how the fit can be improved in such a case.

### 3.2.3 Parameters for the initial conditions of diffusion

The following parameters have no influence on the as-implanted B profile. They fix the point-defect distribution and determine which part of the silicon is considered as amorphous after the implantation:

- **damage=+1** switches on the ‘damage+x’ model. The concentration of point defects after implantation is the product of the as-implanted dopant concentration and a factor (\( \text{ifactor} \) for interstitials and \( \text{vfactor} \) for vacancies).

- **ifactor** scales the initial distribution of interstitials in the damage+x model. It is a very important parameter for transient-enhanced diffusion (TED). Increasing \( \text{ifactor} \) increases the TED of boron. \( \text{ifactor} \) depends on the implantation energy and dose. For high B energies and low doses, \( \text{ifactor} \) is close to 1. For low B energies and high doses, \( \text{ifactor} \) is low.

- **vfactor** scales the initial distribution of vacancies in the damage+x model. Vacancies are not important for B diffusion. By DIOS default, \( \text{vfactor} = \max(\text{ifactor} - 1, 0) \).

- **amorphization=mcdamage** means that the damage accumulated during a Monte Carlo simulation is used to determine which part of the silicon is amorphous after the implantation. With \( d_{acc}=0.1 \) and \( d_{crit}=1 \), the damage created by B implantation is usually insufficient to create an amorphous layer.

### 3.3 Boron implantation parameters (tables)

In the Advanced Calibration file `calib_par_85_tables.cmd`, the relevant implantation entries for B implantation are:

```plaintext
impl:(damage=+1, fitasimplanteddose=off, function=undefined)
impl:(vfactor=0, afactor=1, amorphization=hobler)
impl:(ifactor=$energy/($energy+0.8)*(2e15+$dose)/(2e15+10*$dose)*1e17/(1e17+$energy*$dose))
impl:($channel)
#if $dose < 2e13
impl:(table="B_1e12-4e13.tab")
#else < 3e14
impl:(table="B_1e13-6e14.tab")
#else
impl:(table="B_16e13-8e15.tab")
#endif
```

The parameters **damage**, **ifactor**, **vfactor**, and **fitasimplanteddose** have the same values as for B implantation with Crystal-TRIM. They have been explained previously.
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The following parameters are different to the file calib_par_85_CTRIM.cmd:

- function=undefined: This switches to analytical implantation. If the name of an implantation table is specified, this table is used for looking up Pearson or dual Pearson parameters.

- amorphization=hobler means that an analytical model developed by Hobler [5] is used to determine which part of the silicon is amorphous after the implantation.

- table="table_name" specifies a lookup table to be used for the calculation of the as-implanted profile. The tables B_1e12-4e13.tab, B_1e13-6e14.tab, and B_16e13-8e15.tab each cover the dose range specified in the table file name. These tables have been generated by fitting dual Pearson parameters to the results of calibrated Crystal-TRIM simulations, as described in [1].

- The line impl:($channel) is explained in the following text.

The line impl:($channel) demonstrates the use of DIOS variables to track the process history. $channel is such a DIOS variable. It is used to take into account the effect of preamorphization on ion channeling. Initially, when the initialization block of a parameter file is executed (see Section 2.3.2 on page 9.7), $channel is set to an empty string. In this case, the line impl:($channel) has no effect. In a Ge implantation or Si implantation step (usually used for preamorphization), an insertion of the Advanced Calibration parameter file will change the variable $channel by the DIOS commands:

```plaintext
set channel=undefined
set channel=si(channelingdose=2e12*$energy/(1+$energy)+5e13/(1+$energy),totaldose=1e14)
```

Here, $energy is the energy of the Ge or Si implantation. The set command is evaluated immediately. Thus, for subsequent insertions of $channel, later changes of the variable $energy have no effect. The line impl:($channel) becomes:

```plaintext
impl:si(channelingdose=2e12*$energy/(1+$energy)+5e13/(1+$energy),totaldose=1e14)
```

$energy is still the energy of the preceding Ge or Si implantation. By this line, the fraction of ions that may channel in silicon is fixed to the ratio channelingdose/totaldose.

The channeling dose suggested by the implantation table is overwritten and in most cases reduced. It does not matter if the parameter totaldose is different from the dose used in the implantation. The maximum fraction of ions described by the second Pearson function is determined by the quotient of channelingdose/totaldose.

After a diffusion, the effect of preamorphization on dechanneling is removed. Thus, for insertion of an Advanced Calibration file with species=diff_special (for diffusion after preamorphization), the lines:

```plaintext
set channel=undefined
set channel=
```

set the variable $channel back to an empty string.

In total, the line impl:($channel) helps to take into account the effect of precedent implantations on ion channeling for analytical implantations. Of course, the method is quite crude. A more accurate treatment of this effect requires the use of Crystal-TRIM for implantation.

To allow a mixed use of calib_par_85_CTRIM.cmd and calib_par_85_tables.cmd, all operations with the variable $channel are performed in both Advanced Calibration files.
3.4 Boron diffusion parameters

For diffusion, both Advanced Calibration files set the same parameters.

The global parameters for B diffusion and activation, which are independent of implantation conditions and valid both after B and BF₂ implantations, are set in the general part of the calibration files in the code lines:

\[
\text{diff:}(\text{si}(\text{b}(\text{modclust} = \text{transient }; \text{c}10 = 2e22 \\
\text{q}(\text{ge} = 125.0), \\
\text{d}0 = 1.25, \text{d}100 = 0.033, \text{d}1\text{D}w = 3.26);) \\
\text{diff:}(\text{ox}(\text{b}(\text{d}0 = 0.01 \text{d}1\text{w} = 3.6)));) \\
\text{diff:}(\text{siox}(\text{b}(\text{stc}0 = 1e27 \text{stcw} = 6 \text{sgw} = 0)));)
\]

Parameters set in combination with all B implantation are:

\[
\text{diff:}(\text{si}(\text{b}(\text{aminit} = 3.5e20)));)
\]

Additional parameters, which depend on the energy of the B implantations, are set in the lines:

\[
\text{diff:}(\text{siox}(\text{b}(\text{sg}0 = 60*\text{sgfac}*(\text{energy} + 1.)/(\text{energy} + 0.3)));)
\]

\#if $\text{energy} >= 5
\text{diff:}(\text{acinit} = 3e17)
\#else
\text{diff:}(\text{acinit} = 3e17 + \text{dose}/5e14* \{1.5e18 - 2.4e17*$\text{energy}\})
\#endif

The lines:

\[
\text{set \text{SG}_B = \text{undefined} } \\
\text{set \text{SG}_B = 60*\text{sgfac}*(\text{energy} + 1.)/(\text{energy} + 0.3)}
\]

in the parameter file section for B implantation are needed only for oxidation-enhanced diffusion (see Section 3.12 on page 9.34). The DIOS variable \text{SG}_B is set to the same expression as \text{diff:}(\text{siox}(\text{b}(\text{sg}0))). This allows at a later time to multiply \text{diff:}(\text{si}(\text{b}(\text{sg}0))) by a correction factor, which depends on the oxygen partial pressure.

In addition, the B TED is also influenced by the interstitial solid solubility \text{si}(\{\text{c}10, \text{c}lw\}). It is not changed for a boron implantation, but it is changed for a low energy As implantation, and for Ge and Si implantations.

The above parameters are discussed in groups in the following sections.

3.4.1 Parameters for boron diffusion and clustering

\text{si}(\text{b}(\text{d}0))\] is the prefactor of the Arrhenius-type diffusivity of positively charged B–I pairs\(^1\). It is the most important diffusion parameter for long-time anneals. The value was lowered from the default because of a disagreement between measurement and simulations for the medium time anneals (60–120 s at 1050°C) of ultra shallow junctions. In these cases, the initial damage distribution has only a very small influence on the profile, and the diffusion is determined by the pair diffusivities and the equilibrium interstitial concentration. Therefore, a reduction of the diffusivities was necessary to obtain a good agreement.

\(^1\) In fact, DIOS multiplies all diffusivities of dopant–interstitial pairs by a so-called interstitial efficiency factor \text{ieffz}, where \(z\) represents one of the charge states mm, m, 0, p, pp. All diffusivities of dopant–vacancy pairs are multiplied by \((1-\text{ieffz})\). These factors are not changed from the default.
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NOTE

For very long-time, high-temperature diffusions (for example, 30 minutes at 1000°C), B diffusion can be underestimated with \( \text{si(b(dip0=1.25))} \). For such conditions, often, better results are obtained with the default value \( \text{si(b(dip0=2.9618))} \).

- \( \text{si(b(di0=0, diw))} \) plays a minor role compared to \( \text{dip0} \). Since it is for neutral B–I pairs, it is more effective in the tail region, while \( \text{dip0} \) strongly dominates B diffusion in highly doped regions.

- \( \text{si(b(q(ge)))} \) describes the influence of high Ge concentrations on B diffusion. A positive value increases B diffusivity in regions of high Ge concentration. The value has been calibrated for Ge preamorphization, but not for B diffusion in epitaxial grown SiGe layers. DIOS uses the formula:

\[
D = D_{\text{unperturbed}} \cdot \exp \left( \frac{0.042 \cdot Q \cdot C_{\text{Ge}}}{kT \cdot 5 \cdot 22 \cdot \text{cm}^{-3}} \right) \quad \text{[Eq. 9.1]}
\]

- \( \text{si(b(modclust=transient))} \) switches on the nonequilibrium formation and dissolution of B clusters.

- \( \text{si(b(cl0))} \) is the prefactor of the Arrhenius-type solid solubility of boron. A high value of \( \text{cl0} \) means that a larger fraction of B can be active for a given total concentration. This has a strong influence on the stability of B clusters in regions of very high B concentration.

- \( \text{si(i(cl0, clw))} \) is the Arrhenius-type solid solubility of interstitials. In the equilibrium clustering model for interstitials, which is used by default, the interstitials that are not bound to dopants are shared between small clusters and free interstitials. A high value of \( \text{cl0} \) increases the share of the free interstitials and leads to a faster dissolution of interstitial clusters. This usually leads to more TED, particularly in the tail region. \( \text{si(i(cl0))} \) is not changed by a B implantation, but it is changed by As, Ge, or Si implantation. Low values of \( \text{si(i(cl0))} \) are used to mimic the slow release of interstitials from extended defect clusters such as <311> defects or loops, which are not simulated explicitly.

### 3.4.2 Parameters for initial activation of boron

- \( \text{acinit} \) is the maximum concentration of active B after the implantation in crystalline regions. The rest of the B is initially put into B clusters. Increasing \( \text{acinit} \) also increases B diffusion, because more B is available for B–I pairs at the beginning of an anneal, when the interstitial supersaturation is highest.

- \( \text{aminit} \) is the maximum concentration of active B after recrystallization of regions that have been amorphized by the implantation.

### 3.4.3 Parameters for dose loss modeling

During anneal, a significant part of B atoms may segregate at the Si–SiO\(_2\) interface, which is invisible for a SIMS measurement. This effect is known as dose loss. The dose loss model is explained in Section 2.6 on page 9.19.

The following parameters are calibrated for dose loss modeling:

- \( \text{ox(b(di0=0.01, diw=3.6))} \) fixes B diffusivity in oxide to a higher value than default. This increase is necessary, because with the default diffusivity, most of the B in oxide would stay on the first mesh point, which gives rise to numerical errors.

- \( \text{siox(b(stc0=1e27, stcw=6))} \) is the flux parameter. The relatively high value ensures that the segregation equilibrium is established quickly for high temperatures.
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- $siox(b(sgw=0))$ is the Arrhenius exponent of the segregation coefficient between Si and oxide.
- $siox(b(sg0=value))$ is the Arrhenius prefactor of the segregation coefficient. It is the most important parameter of the dose loss model used and governs the amount of B that can enter the oxide.

$siox(b(sg0))$ depends on the implantation condition and the process history. The formula is:

$$d = \frac{siox(b(sg0=60*sgfac*(energy+1.)/(energy+0.3)))}{\text{energy}}$$

$sfac$ is initially set to 1, because the initialization block of the parameter files contains a line:

set sgfac=1

After preamorphization by Si implantation, $sgfac$ is permanently reduced:

- set sgfac=undefined
- set sgfac=0.04

This reflects the experimental observation that after preamorphization with Si, the B dose loss is significantly reduced. Such a reduction is not observed for preamorphization with Ge. ISE does not have a theoretical explanation for this experimental finding. The variable $sgfac$ has been calibrated to ten SIMS profiles measured after Si preamorphization, B implantation, and anneal, with all experiments having the same B implantation conditions (500 eV, $5 \times 10^{14}$ cm$^{-2}$). It may be that the formula used for $sgfac$ is not reliable for other B implantation conditions.

### 3.5 BF$_2$ parameters

The parameter settings and model assumptions for BF$_2$ are similar to boron. In particular, all diffusivities are the same as after B implantation. Different values are set for $ifactor$, $acinit$, $aminit$, $siox(b(sg0))$, $dacc$, $dcrit$, $cex2$ and the names of the implantation tables. By default, all information about the distribution of fluorine atoms is discarded after implantation.

The as-implanted profiles are calculated essentially with the same models as for boron. One difference is the damage accumulation and amorphization. For BF$_2$, the amorphization cannot be neglected. For energies less than 10 keV, the parameter values $dacc=0.15$ and $dcrit=0.05$ give the best fit to SIMS profiles.

For the initial conditions of annealing, the following parameters have been calibrated:

- $ifactor=0.06*($energy-0.5) for energies < 17.16 ($ifactor$ approaches 1 at this energy)$
- $ifactor=1$ for energies $\geq 17.16$
- $acinit=3e17$
- $si(b(aminit=1.6e20$/energy**2))$ after preamorphization ($if$ $after\_PAI$)
- $si(b(aminit=3.5e20))$ otherwise

The DIOS variable $after\_PAI$ is used to track the process history. It is 0 initially. In a Ge or Si implantation, it changes to 1. In a subsequent annealing step (insertion of a calibration file with $species=diff\_special$), it is set back to 0.

$siox(b(sg0))$ depends on the implantation condition and the process history. The formula for BF$_2$ implantation is:

$$d = \frac{siox(b(sg0=60*sgfac*(4+$energy)/(1+$energy)))}{\text{energy}}$$
NOTE Setting different values for the same diffusion parameters (for example, \texttt{acinit} or \texttt{siox(b(sg0))}) in subsequent implantation commands leads to problems. This may happen frequently in the simulation of 2D structures with many implantation steps. In general, the parameters set in the first implantation will be overwritten by the second implantation, which can reduce the accuracy of the simulation. Section 5.2 on page 9.54 discusses what to do in such a situation.

3.6 Arsenic parameters

For arsenic implantation, essentially, the same models are used as for B and BF$_2$. Of course, many parameter values are different.

For matching the \textit{as-implanted profiles}, \texttt{dacc} is increased to 0.8 for energies greater than 10 keV in Crystal-TRIM simulations, in order to fit the dose dependence of As channeling. For energies between 5 keV and 10 keV, the formula \[
\texttt{dacc} = -0.2 + \frac{\text{energy}}{10}
\]
is used, which ensures a smooth transition between the region below 5 keV (\texttt{dacc}=0.3, that is, default) and above 10 keV.

The \textit{initial conditions for diffusion} are the following:

\begin{itemize}
  \item \texttt{ifactor=$energy*1e15/(1e15+$dose)+$dose/(1e15+$dose)} for energies < 1 keV
  \item \texttt{ifactor=1} for energies \geq 1 keV
  \item \texttt{vfactor=0.1*energy*energy} for energies \leq 1 keV
  \item \texttt{vfactor=0.1*energy/(20+energy)} for energies \geq 1 keV
  \item \texttt{acinit=4e18*$dose/5e14*$dose/5e14} for energies < 25 keV
  \item \texttt{acinit unchanged} for energies \geq 25 keV
  \item \texttt{si(as{amin=2.5e20})}$^2$
\end{itemize}

Below are the \textit{dose loss} parameters for As. Only \texttt{siox(as(sg0))} depends on implantation conditions:

\begin{itemize}
  \item \texttt{ox(as{d0=0.01, diw=3.6})}
  \item \texttt{siox(as{stc0=1e14, sgw=0})}
  \item \texttt{siox(as{sg0=700/(20+$energy)*($dose+1e15)/($dose+5e14)})}
\end{itemize}

For the As \textit{diffusivities} and \textit{pairing coefficients}, many parameters have been changed with respect to earlier versions of the Advanced Calibration. The following parameters are inserted independently of implantation conditions:

\begin{verbatim}
diff:si(as{modclust=transient
 clurate0=2e13  cluratew=6.9
c10=5.5e+25  clw=1.2
dimm0=800  dimmw=4.75
dim=12
pi0mm=3.6e-30  piwmm=-1.75}
\end{verbatim}

1. Not changing \texttt{acinit} for high energy As implantation avoids the possibility to overwrite the value of \texttt{acinit} set in a B implantation, in the case of a B extension / As halo p-n junction.
2. This value corresponds to the maximum equilibrium carrier concentration of As-doped Si at 920°C (extrapolated from [6]).
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\[
\begin{align*}
    pv00 &= 2 \times 10^{-26} \\
    pv0m &= 2 \times 10^{-26} \\
    dvm0 &= 3. \\
    dv00 &= 0.02 \\
\end{align*}
\]

\(si(\text{as} \{ \text{modclus} = \text{transient} \})\) switches on the nonequilibrium formation and dissolution of As clusters. \(si(\text{as} \{ \text{clurate0}, \text{cluratew} \})\) give the Arrhenius-type rate constant for the formation and dissolution of As clusters. \(si(\text{as} \{ c10, ctw \})\) is the solid solubility.

\(si(\text{as} \{ \text{dim0}, \text{dimw} \})\) and \(si(\text{as} \{ \text{pi0mm}, \text{piwmm} \})\) are Arrhenius-type constants for the diffusivity and the pairing coefficient of \(\text{As}^+\text{I}^-\) pairs. Due to their negative charge, they contribute mostly to the diffusion of highly doped As regions.

\(si(\text{as} \{ \text{dim0}, \text{dvm0}, dv00 \})\) are the Arrhenius-type prefactors of the \(\text{As}^+\text{I}^-, \text{As}^+\text{V}^-, \text{and As}^+\text{V}^0\) pair diffusivity.

\(si(\text{as} \{ pv00, pv0m \})\) are the Arrhenius-type prefactor of the \(\text{As}^+\text{V}^0\) and \(\text{As}^+\text{V}^-\) pairing constants.

The influence of pairing constants on the diffusion of As and other dopants is discussed in Section 4.5.4 on page 9.47. In general it is small, much smaller than the influence of diffusivities. It is largest for high pairing constants and for the case where several dopants are present and compete for the available point defects.

Finally, the interstitial solid solubility is changed by an arsenic implantation with energies less than 25 keV:

\[
diff: (si(\text{i} \{ c10 = 5 \times 10^{22} + 9 \times 10^{23} \times 10^{13}/(10^{13} + \text{dose}) \}))
\]

For a high As dose, \(si(\text{i} \{ c10 \})\) is reduced, which slows down the dissolution of interstitial clusters. This reflects the typical situation that end-of-range defects are formed, which are relatively stable. For low As doses, \(si(\text{i} \{ c10 \})\) is close to its default value 9.45e23. For a more detailed discussion about \(si(\text{i} \{ c10 \})\), see Section 4.5.5 on page 9.47.

3.6.1 Vacancy boundary conditions

Arsenic diffuses with interstitials and vacancies. Consequently, some parameters are also specified for vacancies. For arsenic diffusion, it is important that homogeneous Neumann boundary conditions (BCs) are used for vacancies for silicon surfaces:

\[
\begin{align*}
    \text{diff: } &\text{siox(v(bctyp=homneumann))} \\
    \text{diff: } &\text{sini(v(bctyp=homneumann))} \\
    \text{diff: } &\text{sigas(v(bctyp=homneumann))}
\end{align*}
\]

According to the literature, Dirichlet BCs or natural BCs with high recombination velocities are closer to reality.

The reason for using Neumann BCs for V is the following: Dirichlet BCs would fix the concentration of V0 (neutral V) at the surface. In the DIOS diffusion model, V0 is also in equilibrium with As–V pairs in all charge states. In a region of high As surface concentration, the total number of V at the boundary is pinned to very high values, due to the high As–V pairing constant. Therefore, in the simulation one can effectively have a V injection from the surface, which is not observed experimentally. By this mechanism, Dirichlet BCs can lead to an overestimation of As diffusion in the simulation of USJ formation.

However, investigations are ongoing. ISE plans to test more realistic natural boundary conditions and use additional adjustments of pairing constants or diffusivities to calibrate USJ As diffusion.
NOTE  Changes of point-defect BCs must be performed very carefully because the diffusion of all dopants can be affected.

3.7  Phosphorus parameters

The calibration of P parameters is based on a smaller number of profiles than the calibration of B and As parameters. In the Advanced Calibration file, a standard set of parameters is used for the implantation:
damage=+1, ifactor=1, vfactor=0, and so on. For the diffusion and activation, the following parameters are changed with respect to the DIOS default:

```
diff:(si(p(modclust=no q(as=580)
p10=-1.8e-20 p1w0=-1.125
dim0=0.0026 dimw=3.05
di0=0.7))
siox(p(sg0=50, sgw=0, stc0=1e14))
ox(p(di0=0.01, diw=3.6))
```

`si(p(modclust=no))` switches off the P clustering. All P atoms are available for diffusion. This reflects the experimental findings (in all profiles of the ISE database) that, even for very high P concentrations, P peaks dissolve quickly. It may be possible that for extremely high P concentrations a P clustering must be considered in the simulation.

```
si(p(q(as=500)))
```

increases the diffusivity of P in the presence of a high As concentration. This influence of As on P diffusion has been calibrated with the help of SIMS profiles of annealed samples with As and P co-implantation. ISE has no microscopic explanation for the observed influence. The remainder of the parameters (diffusivities, pairing constants, and dose loss parameters) have already been explained in Section 3.4 on page 9.25 and Section 3.6 on page 9.28.

3.8  Indium parameters

For the as-implanted indium profiles, the parameters `dacc`, `amav`, and `amdev` are calibrated in `calib_par_85_CTRIM.cmd`. `amav` and `amdev` govern the range and the range standard deviation in amorphous region:

```
impl:(dacc=0.7, amav=1.04, amdev=0)
```

The following lines of the Advanced Calibration files are related to In diffusion:

```
diff:(si(in(modclust=transient,
p100=3.5e-27
di00=1.568
di0w=3.5645
dip0=0))
siox(in(sg0=1e5 sgw=0 stc0=1e4 stcw=0)))
implantation:(damage=+1, ifactor=1, vfactor=0)
```

```
diff:(acinit=2e18)
impl:(amorphization=+1, ifactor=1200)
```

```
#if $dose > 2e13
diff:(si(n(di00=0, dip0=0, dv0=0,dvp0=0, dvpp0=0) in(q(n=1.5e4))))
impl(element=N, dose=$dose, energy=$energy, tilt=$tilt,
rot=$rotation, amorphization=no, damage=no,
,$p=5nm stdv=0.8*energy* gamma=-1 beta=5))
#endif
```
The diffusivities $s_i(\text{di}00, \text{di}0w, \text{dip}0)$ of indium-interstitial pairs are derived from [7]. The high segregation coefficient $s_{i0}(\text{sg}0, \text{sg}w)$ and flux parameter $s_{i0}(\text{stc}0, \text{stcw})$ make the In segregation into oxide diffusion limited. This means that all In atoms that diffuse to the Si–SiO$_2$ interface end up in the oxide. The model $\text{amorphization}=+1$ is used only for In, not for any other dopant. It serves to describe the double peak phenomena of In profiles (see Section 3.8.1).

A second peculiarity is the nitrogen implantation statement that is introduced before an indium implantation. Here, nitrogen is not used as real nitrogen, but as a purely technical means of simulation to increase the diffusivity of indium in the surface near region, using the coupling parameter $s_i(\text{n}=1.5e4)$. This is further explained in Section 3.8.2 on page 9.32. The increased diffusivity near the surface is necessary to calculate the indium dose loss accurately. The amorphization and dose loss models used for indium diffusion are described in more detail in [8].

### 3.8.1 Double peak

SIMS profiles that are measured after In implantation and annealing show two In peaks under certain experimental conditions. This double peak phenomenon is not observed for other dopants. It is illustrated in Figure 9.2.

The double peak phenomenon can be caused by a buried amorphous layer generating special initial conditions for diffusion, or by defect bands located at the ac-interface. Noda [9] assumes that defects concentrated in bands close to the ac-interfaces are mainly responsible for the double peak phenomenon. In this case, indium is trapped and deactivated at the defects, forming a peak in the region of the highest defect concentration.

In the Advanced Calibration model, the double peak is caused by differences in the initial conditions for diffusion in crystalline and amorphous layers. In the amorphous layer, recrystallization renders a high initial active concentration of indium (by default, $s_i(\text{aminit}=5e22)$) and a low interstitial concentration, whereas in the crystalline part, the initial indium activation is moderate ($\text{acinit}=2e18$) and the initial concentration of interstitials from implantation damage is high. The interstitials diffuse very quickly into the former amorphous layer, where the indium is already active and ready for pairing. In this way, indium diffusion in the amorphous layer is much higher than in the crystalline part.

The model $\text{amorphization}=+1$ is used to create a buried amorphized layer for high indium doses. In this model, the amorphization is calculated as the product of the as-implanted dopant concentration and $afactor$. 
(afactor=1200). Regions in which the amorphization is higher than threshold (by default, threshold=1.15e22) are treated as amorphous and have the corresponding initial conditions for diffusion. In other words, with the parameters selected, the usually buried region in which the as-implanted indium concentration is higher than 1.15 × 10^{22}/1200 cm^{-3} is treated as amorphous.

In contrast, when using the standard amorphization model (amorphization=mcdamage or hobler), the amorphized layer is not a buried layer but moves from the silicon surface to some depth. In this case, one can obtain only the peak at greater depths instead of the two peaks. This situation is observed experimentally in samples that are amorphized by Ge implantation before In implantation.

In the simulation, the sharp transition between amorphous and crystalline regions leads to a spike shape of the In peaks.

### 3.8.2 Indium dose loss

In the indium SIMS profiles for energies lower than 150 keV, an anomalous dose loss behavior is observed [8]. The indium peak concentration in silicon after annealing does not scale linearly with the dose. Instead, for low energies (approximately 50 keV), increasing the indium dose at levels above 3 × 10^{13} cm^{-2} mainly adds to the indium dose in oxide, while the indium concentration in silicon is hardly changed.

A physical reason for this could be that dislocation loops and other defects to which a segregation of indium is possible cause an enhancement of diffusion. Alternatively, it may be that indium diffuses very quickly at the boundaries of crystalline–amorphous pockets, which appear after implantation especially between the surface and the first ac interface, or that indium is swept out during epitaxial regrowth of the amorphized layer.

For the simulation, this means that either the parameters of the boundary conditions (segregation coefficients, flux parameters) or the diffusivities show a special dependency on the dose (concentration). The dose loss is modeled by segregation at the oxide–silicon interface. With the parameters used, the dose loss is diffusion limited. This means that only by increasing the diffusivity in silicon can there be an increase in the dose loss. Thus, it is necessary to increase the diffusivity in the region close to the surface.

To increase the diffusivity close to the surface, an artificial immobile impurity (nitrogen) is used and the In diffusivity is coupled to the N concentration. In this way, it is possible to change the diffusivity in a specific region without introducing a new material. N was chosen because it is electrically neutral and usually not used in process simulations.

The parameters for the artificial N implantation and N–In coupling, $\text{si(rp=5nm stdv=0.8*\$energy\text{nm} gamma=-1 \ beta=5), si(in(q(n=1.5e4)))}$ are calibrated for In energies between 50 and 150 keV and doses between $2 \times 10^{13}$ and $1 \times 10^{14}$ cm^{-2}.

### 3.9 Antimony parameters

The Crystal-TRIM implantation parameters for antimony (Sb) implantation are:

```plaintext
impl:(dacc=1, dcrit=0.2, amav=0.93)

# if $\$energy < 30.0
impl:(amdev=0.14)
# endif

# if $\$energy > 29.999
# if $\$energy < 120.001
```
All of these parameters have been explained in Section 3.2 on page 9.21 and Section 3.8 on page 9.30.

The diffusion parameters for Sb are:

```
diff:(ox(sb(di0=6.4,diw=4.58)),
  oxgas(sb(stc0=5e4)),
  siox(sb(sg0=2)),
  si(sb(modclust=transient,
     cl0=1.25e21,clurate0=2.4e6,cluratew=4.5,
     dv00=0.2568)))
diff:(acinit=1e16)
```

The diffusivity of Sb in oxide is taken from the literature [10]. Sb diffuses predominantly with vacancies. It displays almost no TED. Significant diffusion of Sb occurs only for long-time, high-temperature annealing.

**NOTE** The calibration of Sb parameters has been performed for Sb energies between 50 and 150 keV. No USJ Sb profiles have been used for calibration.

### 3.10 Germanium parameters

As Ge diffuses slowly and is not electrically active, the accuracy of the Ge profile is less important than the accuracy of the dopant profiles. No calibration is necessary for the parameters that determine the Ge distribution. The standard models (damage=+1, ifactor=1, vfactor=0, and so on) are used for damage generation.

To determine the amorphization created by Ge implantation, the following parameters are changed from the DIOS default:

```
impl:(threshold=5e21/(1+$energy/(500.0, particles=5000))
#endif

#if $energy > 120.0
impl: (amdev=0.05, particles=3000)
#endif
```

The following two lines are used to reduce the channeling in subsequent (analytical) implantations:

```
set channel=undefined
set channel=si ( channelingdose=2e12*$energy/(1+$energy)+5e13/(1+$energy),
totaldose=1e14)
```

In addition, a Ge implantation has some effect on diffusion, which are coded in the lines:

```
set after_PAI=undefined
set after_PAI=1
set PAI_cl0=undefined
set PAI_cl0=diff: (si (cl0=3e22*2.5e29/(2.5e29+$dose*$dose)+1.9e37/ (2e13+$dose)*5+$energy/$energy)))
```

The DIOS variable after_PAI is used only for BF$_2$ implantation. The initial active concentration of B in amorphous regions is reduced if the BF$_2$ implantation follows a Ge implantation.
The variable PAI\_cl0 is used to reduce the Arrhenius prefactor of the solid solubility of interstitials, \( si(i(cl0)) \), in all diffusion steps that are after a Ge implantation. PAI\_cl0 is used in order to ‘not forget’ the value of \( si(i(cl0)) \) set in the Ge implantation, even when it is overwritten, for example, by a subsequent As implantation.

Before diffusion, following PAI and dopant implantation, the user is supposed to insert an Advanced Calibration file with the setting `species=diff_special` that will insert the line `$PAI\_cl0`, which sets the calibrated value of \( si(i(cl0)) \).

Physically, the reduced value of the interstitial solid solubility reflects the influence of dislocation loops, which are usually formed after preamorphization. The release rate of interstitials from a band of dislocation loops is relatively small, and the loops are quite stable.

Finally, as mentioned in Section 3.4 on page 9.25, a high Ge concentration can change the diffusivity of boron. In the Advanced Calibration, the parameter \( si(b(q(ge=125))) \) increases the B diffusion in regions of high Ge concentration. This parameter has been calibrated for Ge implantation, but not for epitaxially grown SiGe layers. A similar diffusion enhancement has not been observed for preamorphization by Si implantation.

### 3.11 Parameters for Si implantation

The parameters for Si (interstitial) implantation are very similar to those of Ge (see Section 3.10 on page 9.33). The main difference is that `ifactor` must be set to 0. With `ifactor=1`, two interstitials per implanted silicon atom would be obtained.

A second difference is that the B segregation into Si–SiO\(_2\) is reduced if B or BF\(_2\) is implanted after a Si implantation. This is reflected by the lines:

```plaintext
set sgfac=undefined
set sgfac=0.04
```

The DIOS variable `sgfac` is used in the calculation of the B segregation coefficient (see Section 3.4.3 on page 9.26).

### 3.12 Oxidation-enhanced diffusion (OED)

During oxidation, the equilibrium concentration of interstitials is increased at the oxidizing surface, as a function of the progression speed of the Si–SiO\(_2\) interface. For small implantation energies, the oxidation-enhanced diffusion (OED) effect may change because a significant number of dopant atoms can be trapped at the Si–SiO\(_2\) interface and change the interface properties. The OED parameters are adjusted by:

```plaintext
diff:(si(i(pox=2.7e-4 potox=-2)))
```

The influence of these parameters on increasing the equilibrium interstitial concentration at the surface is described by the OED factor:

\[
\text{OED factor} = \left( 1 + F_{\text{ox}} \cdot F_{\text{dop}} \left( \frac{n_{\text{ox}} \cdot n_{\text{D}}} {1 \text{ Å/min}} \right)^{p_{\text{ox}}} \right)
\]  

[Eq. 9.2]
with:

\[ F_{\text{dop}} = \frac{m_2 + m_1 + 1 + m_1 + m_2}{m_2 q^2 + m_1 q^1 + 1 + m_1 q^{-1} + m_2 q^{-2}} \]  

[Eq. 9.3]

and:

\[ q = \left( \frac{\text{n}}{\text{n}_i} \right)^{\text{PotOx}} \]  

[Eq. 9.4]

\( si(i(\text{pox0})) \) is the Arrhenius prefactor of the exponent \( P_{\text{ox}} \) in [Eq. 9.2]. \( si(i(\text{potox})) \) is used in [Eq. 9.4] and governs the influence of Fermi level on the OED. The formulas are explained in the DIOS manual.

By DIOS default, \( si(i(\text{potox}=2)) \), that is, the sign of \( \text{potox} \) is different. However, with a positive value of \( si(i(\text{potox})) \), it is impossible to describe the doping dependence of the OED.

**NOTE**  
The calibration of \( \text{pox0} \) and \( \text{potox} \) is based only on a relatively small number of SIMS profiles for spike anneals or 10 s RTAs. Do not expect a very accurate description of OED for all kinds of oxidation conditions.

During OED, the segregation coefficient of B is reduced by the formula:

\[
\text{diff:}(\text{si:ox}(\text{B}(\text{sg0}=\text{SSG_B}*(0.0005+\text{sp2})/(0.0005+2.2*\text{sp2}))))
\]

where \( \text{SSG_B} \) is the value of \( \text{sg0} \) in inert atmosphere and \( \text{sp2} \) is the partial pressure of oxygen in the oxidizing atmosphere.

The above code line is executed when a calibration file is inserted with the specification \( \text{species=diff_special} \). Thus, before each oxidation step, one should insert the calibration file with \( \text{species=diff_special} \) and set the DIOS variable \( \text{sp2} \) to the oxygen partial pressure [atm]. After oxidation, the user should switch back to the parameters for inert atmosphere, by inserting a calibration file with \( \text{species=diff_special} \) and \( \text{sp2}=0 \).
4.1 Equation and model system of process simulation

Advanced Calibration is based on the following selection of implantation and diffusion models:

- Pair diffusion framework: In silicon, the diffusing species are point defects (interstitials and vacancies), and pairs of a dopant atom and a point defect.
- Monte Carlo simulation of all implantations (with `calib_par_85_CTRIM.cmd`) or use of analytical tables, which have been calibrated to the results of Monte Carlo simulations (with `calib_par_85_tables.cmd`).
- Damage+x model for the initial interstitial and vacancy distribution.
- Equilibrium model for the clustering of interstitials (no distinction between 311, boron interstitial clusters, and other cluster types).
- First-order reaction equations for dopant impurities: There is only one reaction equation per impurity, which governs the relationship between active and total concentrations.
- Dopant segregation at interfaces.
- Dopant diffusion in all materials.
- Dose loss model based on segregation into oxide layer on top of silicon.

4.2 Experimental data

The main source of experimental data used for the Advanced Calibration calibration is a database of more than 1000 SIMS profiles, most of which are related to state-of-the-art USJ technology. In addition, some SRP profiles and sheet resistance measurements were used to study dopant activation and dose loss.

A part of this database was designed in collaboration with Applied Materials, Inc. as a systematical approach to calibrate process simulation for advanced CMOS technology [11]. The experimental data was produced from Quantum™ implant and Radiance™ RTP systems and are available as a part of the TCAD Fab Package, which is a joint product of ISE and Applied Materials. The TCAD Fab Package also provides a professional calibration platform for further fine-tuning of process physics parameters. A data sheet on the Fab Package can be found at [http://www.ise.ch](http://www.ise.ch) or [http://www.ise.com](http://www.ise.com).

SIMS profiles may show some differences to the real dopant distribution, even when they are measured very carefully. These differences are inherently related to the SIMS technique. In particular, SIMS profiles may show two typical errors:

- In the first few nanometers from the Si surface, the signal is not always stabilized and the SIMS profile is less reliable.
- Very steep profiles (steepness > 1 decade per 2 nm) are usually smeared out during SIMS measurements.

The SRP profiles for USJ are less reliable than SIMS profiles. However, they can be used to monitor the activation or deactivation of dopants during annealing. Sheet resistance data is used in some cases (for example, Sb annealing) to calibrate the activation process of dopants. For very high dopant concentrations in
USJ profiles, the fraction of activated dopants does not solely determine the sheet resistance. In addition, the mobility of electrons and holes is reduced by the presence of the dopant atoms and may depend on process conditions. In this case, the effect of dopant activation and charge carrier mobility cannot be fully separated with only sheet resistance measurements.

## 4.3 Calibrating implantation with Crystal-TRIM

In the Monte Carlo code Crystal-TRIM, the following parameters were used to calibrate the as-implanted profiles:

- Electronic stopping: \( c_{\text{ex1}}, c_{\text{ex2}} \)
- Damage accumulation: \( d_{\text{acc}} \)
- Amorphization/damage saturation: \( d_{\text{crit}} \)
- Free path length in amorphous Si: \( a_{\text{amav}}, a_{\text{amdev}} \)

In addition, the parameter \( \lambda \) can be used to adjust the average path length in crystalline silicon. This parameter is probably needed for an accurate calibration of high-energy B implantation, but it is not yet used in the Advanced Calibration.

In principle, the above parameters can be separated in a three-step calibration:

1. For very low doses (in the case of B implantation also for medium doses), the damage accumulation has only a small effect on the as-implanted profiles. The electronic stopping is \( (c_{\text{ex1}}, c_{\text{ex2}}, \lambda) \) calibrated.
2. \( d_{\text{acc}} \) is adjusted with SIMS profiles for medium doses, which are still too low for amorphization.
3. \( d_{\text{crit}}, a_{\text{amav}}, \) and \( a_{\text{amdev}} \) are only relevant for very high doses or preamorphization.

The implantation calibration is now discussed according to these steps. The main focus is an accurate description of ion channeling.

### 4.3.1 Electronic energy loss

Crystal-TRIM uses the parameters \( c_{\text{ex1}} \) and \( c_{\text{ex2}} \) in a modified Oen–Robinson formula for the electronic energy loss in a binary collision [3]:

\[
\Delta E_{\text{el}} \sim \frac{Z_{\text{BL}} \cdot \exp(-C_{\text{el}} \cdot 0.3 \cdot R_{\text{d}}(E,P)/a)}{\frac{1}{2\pi} \int_0^{P_{\text{max}}} \exp(-C_{\text{el}} \cdot 0.3 \cdot R_{\text{d}}(E,P)/a) dp} \quad \text{[Eq. 9.5]}
\]

where \( R_{\text{d}}(E,P) \) is the distance of closest approach in a binary collision. The function \( Z_{\text{BL}} \) is the ZBL electronic stopping cross section [12], which is successfully used in the simulation of ion implantation into amorphous solids in the standard TRIM program [13]. \( P \) is the impact parameter and \( P_{\text{max}} \) is the maximum impact parameter in the Crystal-TRIM binary collision code. The fit parameter \( C_{\text{el}} \) takes the value of either \( c_{\text{ex1}} \) for directions close to the \(<110>\) direction or \( c_{\text{ex2}} \), otherwise.

According to this formula, the electronic energy loss is reduced for large impact parameters, as is the case of channeling ions. This reduction can be refined with the parameters \( c_{\text{ex1}} \) and \( c_{\text{ex2}} \). The values of \( c_{\text{ex1}} \) and \( c_{\text{ex2}} \) may depend on the implantation energy.
Part 9 – Advanced Calibration

4 – Calibration methodology

For implantations into (100) silicon with tilt angle 0 and energies greater than 5 keV, the channeling in the <100> direction predominates, and only a very small fraction of ions are scattered in the <110> direction. For very low energies, it has been shown [14] that the channeling in <110> prevails. For low implantation energies, a fraction of ions can be scattered in the <110> direction when passing a thin layer of native oxide.

In the course of calibrating B and BF\textsubscript{2} profiles, $cex1$ was adjusted to achieve a fit with USJ SIMS profiles for several energies. Then, an energy-dependent fit formula was found, which gives good fits for all low-energy implantations, down to 0.2 keV in the case of boron. The calibration result is illustrated in Figure 9.3 and Figure 9.4, both taken from [11]. According to Figure 9.3, for implantations through 1.5 nm cap oxide, the channeling in the <110> direction becomes dominant for B energies below 1 keV. In Figure 9.4, the calibration of $cex1$ is most relevant for the far tail region because the fraction of ions scattered in the <110> direction is small, but the channeling of these ions is large.

![Figure 9.3](image1.png)

Figure 9.3 Relative importance of <110> channeling with respect to total channeling. Data points are calculated from the depth at which B concentration is $10^{18}$ cm$^{-3}$ for a $10^{15}$ cm$^{-2}$ B implantation with tilt=0. The substrate orientation is <100>.

![Figure 9.4](image2.png)

Figure 9.4 Comparison of a SIMS profile to Crystal-TRIM results before and after calibration for B implantation at 500 eV through native oxide at tilt angle 0 into silicon with 100 orientation. The change of $cex1$ is mainly responsible for the difference. Changing the electronic energy loss results primarily in a bending of the tail in the logarithmic diagram.

---

1. Instead of increasing $cex1$, a similar effect on the profile tail can be obtained by assuming an energy contamination of 2% 2 keV ions. However, the energy contamination of the implanter used was specified to be less than 0.5%.
The correction factor $\lambda$ can be used to shift the peak position of as-implanted profiles. It is the only parameter that is really effective for this purpose. ISE is currently evaluating it for improving the accuracy of high-energy B implantation.

**Figure 9.5** Influence of the DIOs parameter $\lambda$ on as-implanted B profiles; simulations are performed for a $10^{13}$ cm$^{-2}$ B implantation with energy=120 keV and tilt=7

### 4.3.2 Damage accumulation (dacc)

**Figure 9.6** Influence of dacc on tail of an as-implanted Sb profile (100 keV Sb, dose $10^{14}$ cm$^{-2}$, normal incidence, 5.4 nm capping oxide)

During implantation, the ions create crystal damage, which reduces the channeling for subsequent ions. The amount of crystal damage created is multiplied by dacc, a number between 0 and 1, which reflects the recombination of parts of this damage during annealing. Increasing dacc reduces the channeling. By changing dacc, the channeling tail of the profile is shifted, in parallel, in the logarithmic diagram (see Figure 9.4 on page 9.39 and Figure 9.9 on page 9.43). This is different from the tail bending (see Figure 9.4 on page 9.39) that can be tuned with $cex_1$ and $cex_2$. 
\( d_{\text{acc}} \) may depend on the substrate temperature during implantation and the dose rate [15]. For high temperatures and low dose rate, there is an increased chance for Frenkel pair recombination during implantation, which is reflected by a reduced value of \( d_{\text{acc}} \).

The DIOS switch \( D_{\text{Model}} \) determines how Crystal-TRIM deals with the accumulated damage. The best model is the default selection \( D_{\text{Model}}=6 \). In this model, the damage is translated into a probability that the implanted ion is moving in an amorphous pocket [4]. A region where the damage has reached a threshold value \( d_{\text{crit}} \) is treated as completely amorphous for the rest of the simulation.

### 4.3.3 Amorphized regions and damage saturation

#### 4.3.3.1 \( d_{\text{crit}} \)

For the Crystal-TRIM default damage model \( D_{\text{Model}}=6 \), \( d_{\text{crit}} \) is the amorphization threshold. The smaller \( d_{\text{crit}} \) is, the faster a region is considered completely amorphized. Consequently, for very small values of \( d_{\text{crit}} \), the channeling is reduced. The profile tail changes in a way similar to the case of increasing \( d_{\text{acc}} \), but only for doses high enough to reach the amorphization threshold.

With \( D_{\text{Model}}=6 \) and \( \text{amorphization}=\text{mol}\text{damage} \), another effect of changing \( d_{\text{crit}} \) is a change of the thickness of the amorphous layer. The thickness of the amorphous layer is not seen in SIMS profiles of as-implanted samples, but it has a large effect on the initial conditions of diffusion. For example, it is assumed that there are no interstitials in this region after recrystallization and the initial dopant activation is higher in such a region.

Other parameters in addition to \( d_{\text{crit}} \) are available with which the user can forcibly correct the thickness of the amorphous layers: \( a_{\text{factor}} \) and \( \text{threshold} \). To keep the number of parameters reasonably small, \( a_{\text{factor}} \) and \( \text{threshold} \) are not used for B, BF\(_2\), As, P, and Sb implantation in the Advanced Calibration. The thickness of an amorphous layer can be measured by Rutherford backscattering or TEM analysis. Such measurement data was not available for the calibration.

Alternatively, for some conditions, the position of the ac interface can be seen in SIMS profiles as a small hump after a low temperature anneal. The origin of this spike is that the dopants are bound to clusters in the crystalline region, but not so much in the amorphous region, where the recrystallization renders a high active dopant concentration. An example of this hump is shown in Figure 9.7.

![SIMS profile](image)

**Figure 9.7** SIMS profile after BF\(_2\) implantation, 2.5 keV, dose= 5 x 10\(^{14}\) cm\(^{-2}\), and a 30 s anneal at 850°C (the hump at depth of 7 nm shows position of ac interface after implantation)
4.3.3.2 amav, amdev

When a region is amorphized, DIOS has two methods for calculating consecutive binary collisions:

1. Completely random. This is the DIOS default for In, Sb, and Ge. It can be switched on for As, B, BF₂, and P by setting `function=OldCrystalTRIM`.

2. Improved description involving two empirical parameters $\text{amav}$ and $\text{amdev}$. This is the DIOS default for As, B, BF₂, and P.

In the Advanced Calibration, the second method is used for all dopants.

$\text{amav}$ relates mainly to the range in the amorphous layer. $\text{amdev}$ relates mainly to the standard deviation of dopant distribution in an amorphous layer. Its influence is shown in Figure 9.8. The case $\text{amav}=1$ and $\text{amdev}=0$ gives similar results to $\text{function=OldCrystalTRIM}$. For B, As, and P, the DIOS default values for $\text{amav}$ and $\text{amdev}$ depend on the implantation energy.

**NOTE** In DIOS 8.0 and earlier, $\text{amdev}$ was only calibrated for energies greater than 10 keV, but not for energies less than 10 keV. The default values of $\text{amdev}$ for very low energy B and BF₂ implantations caused an overestimation of the ion range for both preamorphization and high BF₂ dose. This is illustrated in Figure 9.8. This problem is solved in DIOS 8.5 and 9.0 by a change to the default values for $\text{amdev}$. Now, $\text{amdev}=0.0275$ for B and BF₂ implantations with a boron energy below 10 keV.

For indium and antimony, $\text{amav}$ and $\text{amdev}$ were changed to improve the fit to the SIMS profiles in the regions of high concentration. This is illustrated for indium in Figure 9.9 on page 9.43. $\text{amav}$ has a similar effect for amorphous regions as $\lambda$ for crystalline regions.

![Figure 9.8](image_url)  
**Figure 9.8** Effect of $\text{amdev}$ on 500 eV B implantation into preamorphized Si. With the DIOS 8.0 and earlier default formula for $\text{amdev}$, the B profile is calculated deeper than in the case without preamorphization (squares). A better result is obtained when fixing $\text{amdev}=0.0275$ (circles; default in DIOS 8.5 and later). In this case, the B peak with concentration $>10^{20}$ cm⁻³ fits the result of the case without preamorphization.
4.4 Calibrating implantation with tables

The implantation tables (Chapter 6 on page 9.59) have been generated with Crystal-TRIM as described in [1]. Many 1D profiles have been calculated with a calibrated Monte Carlo implantation and a high particle number to ensure good statistics. Then, the moments of the analytical formulas (dual Pearson functions) have been extracted from the calculated 1D profiles, using an extended Levenberg–Marquardt algorithm.

All physics is included in the calibrated parameters of Crystal-TRIM. For the creation of the tables used in calib_par_85_tables.cmd, the Advanced Calibration of Crystal-TRIM parameters has been used.

ISE will endeavor to keep the calibration of the tables up-to-date. In principle, with every improvement of the parameters of Crystal-TRIM, a corresponding, improved version of the implantation tables can be generated. However, this requires significant computational resources.

4.5 Calibrating diffusion

4.5.1 Overview

Diffusion and activation processes are more difficult to calibrate than implantation. The pair diffusion model has numerous parameters many of which are difficult to separate. A pure global optimization can result in a good agreement for a large collection of experimental data, but still have a limited predictive power for other process conditions. This is even the case for experimental data as comprehensive as the TCAD Fab Package.

The DIOS default parameters were the general starting point for calibration. Many were taken from publications. Others were calibrated between 1994 and 1997, when the pair diffusion model was introduced.
into DIOS. Finally, there are few default values that are ‘reasonable assumptions,’ which have never been tested against experimental data.

The DIOS default values were applied to the ISE SIMS database. In cases of insufficient agreement with the SIMS data, ISE has tried to improve the agreement:

- With the least changes possible.
- In a way that is consistent with models for USJ annealing in recent literature.

For a successful calibration, order is very important. Some parameters, such as the interstitial equilibrium concentration, have an influence on nearly all profiles. Others, such as the damage+ factor used for a particular implantation condition, affect only a small number of profiles. It is crucial to calibrate the former first and the latter last.

Following this principle, the physical parameters are classified into four groups:

1. The fundamental point-defect parameters affect nearly all diffusion processes. Examples are the diffusivity and charge-state distribution of interstitials. These basic parameters should not be changed without proven necessity because, when they differ for different projects, all other parameters can no longer be compared and similar parameter sets for similar projects are never found.

2. Some parameters affect all diffusion processes for one dopant, in particular, the pair diffusivities. Ideally, these are changed only within large calibration projects.

3. At the lowest level, there are diffusion parameters that depend strongly on implantation and annealing conditions. These include dopant and interstitial clustering kinetics, the initial amount of point defects, the initial activation of dopants after implantation, the effect of F on B diffusion, and the dose loss parameters. Since these parameters can be given different values for different technologies and devices without major consistency problems, they are used most often for various expedient calibrations.

4. Some parameters cannot be extracted from the available SIMS data and these are not used in the Advanced Calibration. They can be used in 2D application projects for improving the fit with experimental data. For example, a simultaneous change of interstitial boundary conditions and the initial amount of interstitials after an implantation may give the same results in 1D, but different results in 2D diffusion.

In the next section, the calibration of various parameters is discussed in the same order as these four groups. Apart from a systematic approach, calibration is mainly trial and error, but a presentation of this is beyond the scope of this documentation.

### 4.5.2 Fundamental point-defect parameters

The fundamental point-defect parameters are:

- Diffusivities of I and V
- Charge state distribution of I and V
- I–V recombination (generation) rate
- Boundary conditions of I and V

In the Advanced Calibration file, only one of these parameters are changed from the DIOS default:

```diff:(siox(V(BCTyp=HomNeumann)) sini(V(BCTyp=HomNeumann)))```
The reason for using homogeneous Neumann boundary conditions for vacancies is discussed in Section 3.6.1 on page 9.29.

### 4.5.3 Pair diffusivities

The diffusivities of dopant point-defect pairs are extracted from SIMS data from so-called long-time anneals, where the damage-enhanced TED can be neglected and the dopant activation is close to equilibrium. To obtain a prefactor and an activation energy of an Arrhenius-type diffusivity, data for high temperature (seconds or minutes > 1000°C) and low temperature (hours < 850°C) is required.

Usually, this must be performed at different doses, background doping levels, and counterdopant implantations in order to obtain the values of the diffusivities of the different charge states. Otherwise, only information about a global value of the diffusivity is obtained. As there is little special data, ISE has relied in many cases on DIOS default values and data from literature for the diffusivities of the different charge states.

Generally, the calibration of diffusivities is performed according to the following scheme. When a good agreement with SIMS profiles is obtained, the calibration is stopped at the earliest possible level:

1. Use DIOS default values.
2. Change the Arrhenius prefactor of the dominant diffusivity (for example, $si(B(dip0))$ in the case of B diffusion).
3. If profiles with high dopant concentration ($N_{dopant} > n_i$) are involved, change the relative contributions of different pair-charge states to diffusion.
4. When SIMS profiles of different temperatures must fit, change the Arrhenius activation energy of diffusivities.

**NOTE** A significant change of activation energy is always accompanied by a change of the Arrhenius prefactor, in such a way, that for a selected temperature the total Arrhenius value is kept constant.

Figure 9.10 on page 9.46 shows the effect of diffusivity changes on ‘long-time’ annealing of a USJ B profile. Using the DIOS default values, boron diffusion is usually overestimated for high temperature anneals of 10–500 s of USJ boron profiles.

The DIOS default values of B pair diffusivities were calibrated to SIMS data [16] (and references therein). In comparison with these old SIMS data and also some new SIMS data with very long-time high-temperature anneals, the B diffusion is underestimated with the TCAD Fab Package parameters. The reason for this inconsistency has not been clarified yet. It may be related to some detail of the experimental conditions, such as the C concentration of the wafer.

Currently, ISE recommends using the TCAD Fab Package parameters for all types of USJ profile. For very long-time high-temperature anneals (such as 30 minutes at 1000°C), ISE recommends that the simulation results are compared with at least one SIMS profile and that adjusting the parameter $si(b(dip0))$ to increase the accuracy of the fit is considered.
4.5.3.1 Effect of charges and doping level

As derived in the DIOS manual, the flux of boron interstitial pairs can be expressed as:

$$\vec{j}_{B-Iz} = -D_{B,Iz} \cdot k_{B,Iz} \cdot \left(\frac{n}{n_i}\right)^{1/z} \cdot \left(\frac{n}{n_i}\right)^{z} \cdot \text{grad}\left(\vec{B} \cdot \vec{i0} \cdot \left(\frac{n}{n_i}\right)^{1/z}\right)$$

[Eq. 9.6]

where, $z$ is the charge of the interstitial in the ($B^{-} I^{+}$) pair, $n$ is the electron concentration, and $n_i$ is the intrinsic electron concentration. In the dilute approximation used by DIOS, the product $D_{B,Iz} \cdot k_{B,Iz}$ is proportional to the DIOS expression $diz0 \times \exp(-dizw/kT)$. Here, $z$ represents one of $p_D$, $p_I$, $0$, $n$, and $m$.

In the above formula, the charge $z$ appears in the term $(n/n_i)^{1/z}$ and $(n/n_i)^z$ depends on the doping level. It is approximately 1 for low doping and very high temperatures. For high $B$ doping ($p \sim B^-$), it is approximately $(n_i/B^-)$.

It can be concluded that:

For regions of high B concentration, B diffusion using ($B^{-} I^{+}$) pairs is enhanced by a factor of $B^-/n_i$ due to the effect of charges. Charges have no particular effect on B diffusion using ($B^{-} I^0$) pairs.

An analogous conclusion holds for dopant vacancy pairs and donor atoms. In the latter case, $B^-$ must be replaced by $As^+$ or $P^+$.

For calibration, the above conclusion has an important implication. The user can increase the diffusion specifically in highly doped regions by increasing the diffusivities for acceptors paired with positively charged point defects or donors paired with negatively charged point defects (see also Figure 9.10 on page 9.46). This calibration method is even more effective when using pairs with double-charged point defects as, for example, in the As parameter diff: {si:{as:{dimm0}}}. 

---

### Figure 9.10
Comparison of simulation results with different diffusivity values for B–I pairs for a 60 s, 1050°C anneal after 2.5 keV BF2 implantation. B diffusion is overestimated with the default diffusivities (circles). The balance between $dip0$ ($B^{-} I^{+}$ pairs) and $di00$ ($B^{-} I^0$ pairs) can be used to adjust the ratio between diffusion in highly doped regions and in the tail (see steepness of tail of the red and the blue curves). 

- **dip0=2.916, di00=0.037, di0w=3.46** (default)
- **dip0=1.25, di00=0.033, di0w=3.26** (Adv. Calibration)
- **dip0=0.000, di00=0.150, di0w=3.26**
For spike annealing conditions, As-profiles often show an almost ‘rectangular’ profile, that is, a very flat high-concentration region followed by a very steep junction. In the Advanced Calibration, the parameters \( \text{diff:si}\{\text{as}\{\text{dim0, dimw, pi0mm, piwmm}\}\} \), which are not used in DIOS default, are introduced to enhance As diffusivity in the highly doped regions and simulate this characteristic shape of As profiles.

### 4.5.4 Pairing constants

DIOS uses the pair diffusion model in the *dilute approximation*. The DIOS diffusivities are, in fact, effective diffusivities, which are proportional to the product of the real pair diffusivity and the pairing constant. Increasing the pairing constant automatically reduces the real pair diffusivity by the same factor, such that the effective diffusivity stays the same.

As long as the pairing constants are small, their actual value has virtually no effect on the simulation result. ‘Small’ means that the concentration of pairs is much lower than the concentration of dopants. Most pairing constants used by DIOS are small in this respect, but there are exceptions, such as the pairing constant \( \text{slp}\{\text{pi00, piw0}\} \) and the pairing constants for As-V pairs.

If the pairing constant is large, a significant fraction of dopants and point defects can be in dopant point-defect pairs. This has several consequences:

1. If the pairing constant is further increased by some factor \( x \), the number of pairs cannot increase by the same factor, because there are not enough dopants available. However, the real pair diffusivity is divided by \( x \), and thus, as a total effect, the dopant diffusion is reduced.

2. The point defects are strongly bound to the dopants and, therefore, are prevented from diffusing away to other regions of the device. This can be important for the simulation of marker layer experiments and, for 2D simulations, for example, when considering the effects of point defects from source/drain regions of a MOSFET on the diffusion in the region under the gate.

A ‘correct’ calibration of the pairing constants is almost impossible, because they are usually too small to play a major role and because their influence can hardly be separated from the effect of other parameters. In the Advanced Calibration, every effort was made not to change too many of the default values of DIOS. The pairing constants were only changed in cases where the interplay of several dopants (for example, As and P co-diffusion) could be improved.

### 4.5.5 TED due to point defects from implantation damage

#### 4.5.5.1 Interstitials

No attempt is made to simulate the clustering of interstitials and the formation of 311 defects and loops using a set of reaction equations. Instead, simple models are chosen to describe the time and temperature dependence of TED after implantation. For this purpose, it is satisfactory to have a model that gives a sufficiently accurate description of the interstitial supersaturation.

Using the default equilibrium clustering model for interstitials proved to be sufficient for achieving good fits of the dopant distributions to the SIMS profiles. This model has much better convergence properties in DIOS than transient interstitial clustering or release of interstitials from traps. A calibration of ifactor in the damage+x model allows for tuning the total amount of TED due to implantation damage.
The time and temperature dependence of TED can be tuned by changing the values of the interstitial solid solubility $s_i(i|c_{i0}, c_{iw})$ (see Figure 9.11).

Figure 9.11 Time evolution of interstitial concentration at depth of 15 nm for a 1000°C anneal after B implantation (1 keV, 5 x 10^{14} cm^{-2}). A low solid solubility $s_i(i|c_{i0})$ of interstitials results in a slower TED. The black line shows the simulated temperature ramp.

Whether a fast dissolution of interstitial clusters increases the diffusion depends on the time dependence of the dopant activation:

**4.5.5.2 Case 1**

If all dopants are active from the beginning (this is usually the case in the tail region), a fast dissolution of interstitial clusters (high value of $s_i(i|c_{i0})$ during ramping-up) increases the diffusion. Interstitials released from clusters at lower temperatures are more effective in terms of dopant transport. Initially, this seems paradoxical.

The reason is that the product of interstitial diffusivity and interstitial equilibrium concentration has a higher temperature dependence than the B–I pair diffusivity in the so-called dilute approximation used by DIOS. The decrease of B–I pair diffusion at low temperature is more than overcompensated by the facts that:

- Free interstitials stay longer inside Si because of their lower diffusivity at low temperature.
- The B–I diffusivity enhancement per excess interstitial is higher at low temperature because the equilibrium concentration of interstitials is lower.

**4.5.5.3 Case 2**

Most dopants are clustered at the beginning of TED. In this case, a rapid release of interstitials from clusters may have the effect that most interstitials are gone before the dopant atoms become active. As a result, increasing $c_{i0}$ decreases the diffusion from high concentration (stable clusters) regions, but may still increase the diffusion of the tail.
4.5.5.4 Vacancies

Since homogeneous Neumann boundary conditions are used for vacancies, the vacancies from implantation damage cannot escape the bulk silicon except by recombination with interstitials. For this reason, in the damage+x model, $v_{\text{factor}}$ must be either less than $i_{\text{factor}}$ or equal to zero.

**NOTE** For some elements (for example, B, BF$_2$, Sb), $i_{\text{factor}}=2$ and $v_{\text{factor}}=1$ are the default values in the damage+x model. These default values are incompatible with using homogeneous Neumann boundary conditions for vacancies, because the large number of vacancies cannot recombine at the surface.

4.5.6 Dopant activation

The transient clustering model $s_i(A_j(\text{modclust} \to \text{transient}))$ is used for all dopants except for P (see Section 3.7 on page 9.30). In this model, the solid solubility $s_i(A_j(\text{cl0,clw}))$ determines the equilibrium concentration of active dopants, and the clustering rate $s_i(A_j(\text{clurate0,cluratew}))$ determines how fast this equilibrium is reached. The initial activation is given by $a_{\text{cinit}}$ in crystalline regions and $s_i(A_j(\text{aminit}))$ in regions that are recrystallized after amorphization during ion implantation.

4.5.6.1 $a_{\text{cinit}}, a_{\text{aminit}}$

By default, $a_{\text{cinit}}$ is low and $a_{\text{aminit}}$ is high ($5 \times 10^{22}$ cm$^{-3}$). Both parameters are crucial for the initial stage of TED. Figure 9.12 shows the influence of $a_{\text{cinit}}$ for a B USJ spike anneal, and it is clear that $a_{\text{cinit}}$ limits the number of dopants available for TED. Comparing the curves for $a_{\text{cinit}}=1e18$ and $a_{\text{cinit}}=1e16$ shows the typical influence of $a_{\text{cinit}}$. For the first moments of TED, when the interstitial supersaturation is highest, only the initially active atoms can diffuse. While the clustered dopant atoms are still immobile, the initially active atoms diffuse into the tail region.

Figure 9.13 on page 9.50 shows the influence of $a_{\text{aminit}}$ after an amorphizing BF$_2$ implantation. The tendencies are the same as for $a_{\text{cinit}}$. The main difference is that $a_{\text{aminit}}$ always has a high value because solid phase epitaxy renders a high activation of dopants.
4.5.6.2 \( cl_0, cl_w \)

The solid solubility is accurately known from literature. Therefore, in the course of calibration, changes from the default values should be small. Changes are very effective for conditions with very high dopant concentration, especially for USJ profiles with high implantation dose.

For calibration, the solid solubility can be used to improve the description of the influence of doping concentration on clustering.

In Figure 9.14, it is shown that a change of \( cl_0 \) is much more effective for high implantation doses than low doses. \( cl_w \) can be used to calibrate this effect for several temperatures.

![Figure 9.14: Effect of \( cl_0 \) on B USJ annealing for high and medium implantation doses. The anneal is 5 s at 1050°C; B energy is 0.5 keV. For the high implantation dose, the change of \( cl_0 \) is more effective.](image)
4.5.6.3 clurate0, cluratew

The clustering rate determines the time in which the dopant clustering reaches equilibrium. Its effect on diffusion depends on the initial activation of dopants. If the initial activation is above the solid solubility (as may be the case, for example, after solid phase epitaxy), a low clustering rate maintains a ‘superactivation’ of dopants. In the opposite case, a low clustering rate preserves a low dopant activation for a long time. For the clustering timescale, the most important issue is whether dopant clustering is faster or slower than the disappearance of the excess interstitials present after implantation. A comprehensive discussion of all conditions is beyond the scope of this documentation.

4.5.6.4 SRP profiles and sheet resistance

SRP profiles and sheet resistance measurements provide additional information on dopant activation and can be used for the calibration or testing of the clustering models. Unfortunately, for USJ profiles, the SRP technique is less accurate (and less direct) than SIMS.

For example, the clustering rate of Sb was calibrated with sheet resistance data. For Sb, a calibration of the clustering rate with SIMS is almost impossible because Sb diffuses very slowly and shows little TED. Sheet resistance data was available for a number of annealing conditions after $10^{13}$ or $10^{14}$ cm$^{-2}$ implantation. For the shortest anneal times and lowest annealing temperatures, the sheet resistance was higher than for the other conditions, reflecting a lower dopant activation. This behavior was calibrated by choosing a low initial active concentration $acinit$, and refining $clurate0$ and $cluratew$ until a good match with measured sheet resistances was obtained.

4.5.7 Dose loss parameters

During annealing, a part of the implanted dose may diffuse out of the silicon. It will be missing in a subsequent SIMS profile, which is called dose loss. For As, it has been shown that most of the ‘lost’ As is captured in the interface between Si and SiO$_2$ within a few atomic monolayers [2]. For other dopants, it may be the same.

Fluorine is also known to be lost during annealing. ISE believes that a part of F comes to rest at the Si–SiO$_2$ interface and increases the capability to build in B. This is the clearest explanation for the experimental fact that the dose loss is higher after BF$_2$ implantation than after B implantation.

In the Advanced Calibration, dose loss is modeled by dopant segregation into SiO$_2$. The first 1–2 nm of oxide substitute the capability of the interface to capture atoms. In 2D simulations, care is required to avoid undesired effects from this segregation model (for example, penetration from polysilicon to silicon through the gate oxide). This is explained in detail in Section 2.6 on page 9.19.
Figure 9.15 shows the effect of dose loss for a long-time, high-temperature anneal.

**Figure 9.15** Effect of segregation coefficient on B profile after BF$_2$ implantation with $E = 2.5$ keV, dose $= 5 \times 10^{14}$ cm$^{-2}$ and 4 minutes anneal at 1050°C. The best agreement is obtained for $s_g0=140$. All other simulation parameters are taken from the Advanced Calibration. In the upper-left corner, it is clear that a very high B concentration is established in the SiO$_2$ layer.
The Advanced Calibration file can be considered a good starting point for 2D simulations (especially for CMOS and SOI CMOS devices) and can reduce the effort for calibration. However, regarding the finite accuracy and the known limitations, it cannot fully replace a calibration of process calibration for 2D applications. With a customized process calibration, the accuracy can always be further increased for any technology of interest. A customized calibration of process and device simulation models can be requested from ISE in the frame of customer service projects.

The current version of the Advanced Calibration parameter set is designed for USJ applications (for example drain extension for deep submicron transistors). For other types of processes, for example long-time high-temperature anneals, the accuracy of these parameters is limited. In this section, the known limitations of the Advanced Calibration parameters are discussed.

To further improve the Advanced Calibration, ISE appreciates any feedback from users, in particular, on the accuracy obtained with the parameter files for different process conditions.

### 5.1 Computation time

#### 5.1.1 Implantation

Monte Carlo simulations can be very time-consuming in 2D. If CPU time is critical, reduce the number of particles (for example, to 3000) and reduce the number of particle splits (for example, maxSplit=(4,0,0) for halo implantations).

In 2D application projects, where several variants are studied, it is usually sufficient to run all Monte Carlo simulations only once. After saving the as-implanted profiles in the DIOS .exp format, a CPU time–expensive implantation can be replaced by a fast load statement.

For this workaround, in order to imitate the damage+1 model, also load interstitial and vacancy profiles and – in the case of high implantation doses – save and load the dataset amorphization.

Alternatively, the user can switch to analytical implantation with calib_par_95_tables.cmd. These are much faster than MC implantations.

#### 5.1.2 Diffusion

Most models used in the Advanced Calibration have a very good convergence behavior in DIOS. There are no numerical problems with selected models in 1D and 2D process simulation.

The convergence is usually a bit worse for diffusions in oxidizing atmosphere, but still quite good. In cases, where the oxide growth and the oxidation-enhanced diffusion can both be neglected, it may be useful to consider speeding up the simulation by using an inert atmosphere.

There may be cases, where the transient dopant clustering model for As increases the simulation time. Thus, in case of insufficient convergence behavior, it is worthwhile testing if the simulation can be accelerated by
replacing \texttt{diff:(si(as(modclust=transient)))} with \texttt{diff:(si(as(modclust=equilibrium)))}, and if such a replacement can be performed without significant changes of the dopant distribution and activation, at least for some process steps.

5.2 Consistency of parameters

Many parameters depend on the implantation conditions. This is no problem for parameters such as \texttt{ifactor}, which have a meaning only for a single implantation step. However, if a diffusion parameter is set to different values in several implantation steps of a process simulation, there may be a severe inconsistency problem. In this section, this is discussed for all such parameters of the Advanced Calibration.

5.2.1 \texttt{acinit}

If \texttt{acinit} is set twice in two subsequent implantations with no diffusion in between, the first value will be overwritten by the second. If both values are significantly different, the initial activation of the first profile is wrong, which can lead to consecutive errors.

As a workaround solution to this inconsistency, insert a dummy diffusion step in between the two implantations, for example, in the case of an In halo implantation followed by an As extension implantation:

\begin{verbatim}
... impl(elem=in, dose=1e13, tilt=30, rotation=90, energy=120)
diff:(acinit=2e18)
diff(temperature=500, time=1e-12)
impl(elem=as, dose=5e14, tilt=0, energy=2)
diff:(acinit=4e18)
...
\end{verbatim}

The third line is a dummy diffusion step. The diffusion time is extremely short, thus the dopant redistribution can be neglected. However, this dummy diffusion fixes the initial activation (\texttt{acinit=2e18}) of In before it is overwritten by the initial activation that is to be used for As (\texttt{acinit=4e18}).

If the implantation is performed with Crystal-TRIM, this workaround has the drawback that the implantation crystal damage is removed after the dummy diffusion, which increases the ion channeling in the second implantation.

5.2.2 \texttt{si(i(cl0))}

The Arrhenius prefactor of the interstitial solid solubility depends on the implantation conditions. It is changed from default for As, Ge, and Si implantations. As shown in Figure 9.11 on page 9.48, \texttt{si(i(cl0))} governs the time dependence of the TED.

Using different values of \texttt{si(i(cl0))} in a long process simulation is often not a problem. Typically, most of the interstitials that come from one ion implantation are gone after the first annealing step following the implantation. In this case, there is no reason why \texttt{si(i(cl0))} cannot be changed after the next implantation step.

Again, a consistency problem arises for a halo implantation followed by extension implantation, or vice versa. In this case it is recommended to use the value \texttt{si(i(cl0))}, which corresponds to the extension implantation, because the simulation of ultra shallow profiles needs a higher accuracy.
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After preamorphization by a Ge or Si implantation, a relatively stable damage layer forms at the interface region between amorphized and crystalline silicon, usually consisting of so-called end-of-range dislocation loops. These loops act as a sink of interstitials in the very early stage of TED and as a source of interstitials later [17], thereby retarding the TED. The loops may be present until the end of a fabrication process and dominate the TED timescale. Therefore, after a Ge or Si implantation, the low values of $s_i(i(c10))$ are preserved for the rest of the process.

5.2.3 $s_i(\rho(sg0))$

The prefactor of the Arrhenius-type segregation coefficient of B depends very strongly on implantation conditions. In the Advanced Calibration, $s_i(\rho(sg0))$ is higher for BF$_2$ than for B implantation, it is reduced by a Si implantation and, in addition, it depends on the B (or BF$_2$) implantation energy.

$s_i(\rho(sg0))$ is not only important for the initial phase of annealing, but also for all diffusion steps that follow an implantation. Therefore, overwriting a given parameter value in a subsequent implantation step can cause a significant inconsistency trouble. This may happen, for example, when a process involves several B or BF$_2$ implantation steps.

In such a case, the user should decide in which part of the device the accuracy is most important and make a choice of parameters manually. For example, in a p-type MOSFET with BF$_2$ extension implantation and B source–drain implantation, the accuracy of dose loss modeling is probably more important for the extension region than for the source–drain region. After B implantation, the user can reset the value of $s_i(b(sg0))$ to the value given after the BF$_2$ implantation, by direct insertion of an appropriate statement `diff:(s_i(b(sg0)=...))` in the DIOS input file.

5.3 Accuracy

5.3.1 Definition of ‘good visual fit’

Figure 9.16 on page 9.56 shows two typical cases for the accuracy of simulation. Generally, the agreement between measurement and simulation is sufficient. In the case of as-implanted profiles, the agreement is mostly excellent.

A good visual fit was obtained for nearly all profiles used in the calibration, including the profiles of the TCAD Fab Package. However, this does not mean that the parameter sets and models reflect completely the physical processes relevant for the corresponding process steps. Continual work is necessary to improve the results and to extend the database to more conditions, species, and specially designed experiments, especially to keep up with the latest technologies.
A ‘good visual fit’ means that, on a certain scale of the depth axis and logarithmic concentration axis, the simulated and measured profiles have the same shape and do not show large differences. The scale of the axis corresponds to typical lengths of a deep submicron transistor.

In Figure 9.16, one of the annealed profiles shows a very good visual fit, while the other shows a worse fit, which is barely acceptable. Defining the penetration depth as the depth of the profile at which the concentration equals $10^{18}$ cm$^{-3}$, the accuracy can be quantified slightly more. The difference between measured and simulated penetration depth should be less than 10 nm for all profiles used for calibration. This is a reasonable value that takes into account the measurement error, meshing effects, and uncertainties in the process conditions specified. In evaluating the accuracy, the surface region down to a depth of 5 nm is not included, and the low concentration regions (concentration less than $10^{16}$ cm$^{-3}$) are ignored.

### 5.3.2 Conditions covered by the Advanced Calibration

The Advanced Calibration is based on a database of more than 1000 SIMS profiles. Although this is a large number, not all possible process conditions and parameter combinations are covered. Naturally, the calibrated models are most reliable for such process condition windows, where many profiles were available for calibration and where a good agreement was obtained for these profiles. These include:

- All implantations except:
  - Very high energy implantations (> 400 keV)
  - Medium energy B implantation (not calibrated yet)
  - USJ In implantation
  - USJ Sb implantation
- B USJ annealing in inert atmosphere
- BF$_2$ USJ annealing in inert atmosphere
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- As USJ annealing
- Co-diffusion of B/BF₂ USJ and As halo profiles (typical CMOS fabrication step)
- Co-diffusion of As USJ and B/BF₂/In halo profiles (typical CMOS fabrication step)

The accuracy is also quite good for further process conditions related to typical CMOS processes, such as source–drain annealing (including co-diffusion of P and As), well–channel annealing (including In and Sb channel profiles), and B extension formation after preamorphization by Ge or Si implantation.

The calibration of the oxidation-enhanced diffusion (see Section 3.12 on page 9.34) is based on a relatively modest set of measurements and is probably not very reliable.

The known cases in which the accuracy of the Advanced Calibration is not good are discussed in the following sections.

It is also important to know, what has not been calibrated in the Advanced Calibration. For such models and process windows, the expectations on the accuracy should not be too high. The most important processes that are not treated in the Advanced Calibration are:

- Diffusion in polysilicon
- Diffusion in epitaxially grown SiGe
- Implantation at very high energies (> 500 keV)
- Sb USJ annealing
- Oxidation: For the oxide thickness, the Advanced Calibration uses the DIOS default parameters of the Massoud model.
- Effects of C on diffusion
- Effects of F implantation on B diffusion
- N diffusion in Si and oxide

5.3.3 Known problems I: Dose loss

The dose loss models have been calibrated for conditions typical for USJ formation, for example, for low energy B implantation followed by a spike anneal or RTA. For other conditions, the B dose loss can be overestimated.

5.3.3.1 Low surface concentration of B

When the surface concentration of B is low (for example, in the channel of NMOS devices), B is known to pile up towards the surface. This dopant pileup is destroyed by the high segregation coefficient that is calibrated for high concentration profiles. For such conditions, it may be necessary to replace the dose loss model by the default parameters for $\text{siox}(\text{b}, \text{sg}, \text{sgw}, \text{stc}, \text{stcw})$.

A physical explanation for this could be that there needs to be some minimum amount of B at the Si–SiO₂ interface in order to allow a fast segregation of additional B.
The segregation behavior of B after a medium dose BF₂ implantation is not completely clear. Most probably, the F goes to the Si−SiO₂ interface, where it helps B to segregate into the oxide.

5.3.3.2 Long-time or very high-temperature annealing

In long-time anneals or very high-temperature anneals (for example, 1150°C), the dopant diffusion in the oxide can be overestimated and, consequently, the dose loss is calculated too high with the Advanced Calibration parameters. In addition, it depends on the oxide thickness and will be higher for regions covered with thick oxides than for regions covered with thin oxides.

In such cases, it is best to reduce the diffusivity of the dopants in the oxide to adjust the desired amount of dose loss.

It is planned to overcome this problem in a future release of the Advanced Calibration file, by changing from the conventional segregation model to the new three-phase segregation model. In this model, a part of the dopants can be stored in the interface layer, which provides an easy way to limit the dose loss for very long-time or high-temperature diffusions.

5.3.4 Known problems II: Boron long-time anneals

While the calibrated B diffusivities work well for short- and medium-time RTA of B USJ (for example, 1−60 s at 1050°C), they turn out to be too low for long-time annealing at high temperatures (for example, 60 minutes at 1000°C). Therefore, for such kind of annealing, the DIOS default parameters are a better choice.

The reason for this discrepancy has not been clarified yet.

5.3.5 Known problems III: Dopant activation and deactivation

The parameters of the Advanced Calibration are not very reliable for dopant activation and deactivation. The reason for that is that only a small number of SRP profiles was available for calibration, compared to a large number of SIMS profiles, which contain no direct information on the activation level of the dopants.

In particular, no calibration has been performed for dopant (for example, As) deactivation, which typically may happen at long-time low-temperature process steps at the back end section of chip manufacturing. In addition, Sb deactivation, which plays a role in USJ formation with Sb, has not been considered.

In cases where most of the dopants are active, the sheet resistances are usually well reproduced, when loading the results of DIOS Advanced Calibration in a device simulation with DESSIS. The typical error bars for sheet resistance simulations are ±15%.
As an alternative to the accurate but slow Monte Carlo algorithm for implantation, the user can use analytical implantations. There are implantation tables with Pearson parameters for As, B, BF₂, P, As, In, Sb, and Ge, which are based on calibrated Monte Carlo simulations [1]. They cover the materials silicon, polysilicon, oxide, and nitride. If other materials are present in a device (for example, resist), the DIOS default tables will be used for such materials.

For silicon, dual Pearson functions are used with parameters depending on energy, tilt angle (0–60 degrees), dose, and oxide thickness. For the other materials, single Pearson functions are used with parameters depending on implantation energy and tilt.

All entries are based on fits to Monte Carlo Crystal-TRIM simulations, which have been performed with a high number of particles. Each table covers one implantation species and a limited dose range. Table 9.12 lists the available tables.

### Table 9.12 Tables for analytical implantation

<table>
<thead>
<tr>
<th>Implantation species</th>
<th>Energy range [eV]</th>
<th>Low dose</th>
<th>Medium dose</th>
<th>High dose</th>
</tr>
</thead>
<tbody>
<tr>
<td>As</td>
<td>0.5–400</td>
<td>As_1e12-5e13.tab</td>
<td>As_1e13-8e14.tab</td>
<td>As_2e14-6e15.tab</td>
</tr>
<tr>
<td>B</td>
<td>0.2–480</td>
<td>B_1e12-4e13.tab</td>
<td>B_1e13-6e14.tab</td>
<td>B_16e13-8e15.tab</td>
</tr>
<tr>
<td>BF₂</td>
<td>0.5–400</td>
<td>BF2_1e12-5e13.tab</td>
<td>BF2_1e13-8e14.tab</td>
<td>BF2_2e14-6e15.tab</td>
</tr>
<tr>
<td>P</td>
<td>0.3–400</td>
<td>P_1e12-4e13.tab</td>
<td>P_1e13-6e14.tab</td>
<td>P_16e13-8e15.tab</td>
</tr>
<tr>
<td>In</td>
<td>1.0–400</td>
<td>In_1e12-4e13.tab</td>
<td>In_1e13-6e14.tab</td>
<td>In_16e13-8e15.tab</td>
</tr>
<tr>
<td>Sb</td>
<td>1.5–600</td>
<td>Sb_1e12-5e13.tab</td>
<td>Sb_1e13-5e14.tab</td>
<td>Sb_2e14-1e16.tab</td>
</tr>
<tr>
<td>Ge</td>
<td>1–50</td>
<td>–</td>
<td>–</td>
<td>Ge_5e13-5e15.tab</td>
</tr>
</tbody>
</table>

The first part of the name specifies the implantation species; the second part gives the dose range for which the channeling is described accurately.

In 1D simulations, the tables provide almost the same accuracy as Monte Carlo simulations with Crystal-TRIM. In 2D simulations, where the lateral distribution of dopants can be very important, more accurate results are still to be expected when using Crystal-TRIM.

### 6.1 Using the tables

To use one of the tables, specify its name in the implantation command, according to the implantation species and dose. Examples are:

```plaintext
impl(elem=as, energy=200, dose=1.2e13, tilt=0, table="As_1e12-5e13.tab")
impl(elem=b, energy=20, dose=2e15, tilt=0, table="B_16e13-8e15.tab")
```


