Figure 6: Example 21 - Be and interstitial profiles for Full.coupled anneal of grown-in Be in GaAs.

Figure 5: Example 20 - Be and interstitial profiles for Two.dim anneal with "plus one" model and defect sink/source after Be implant into GaAs.

Figure 4: Example 19 - Interstitials (created by "plus one" implant), before and after anneal in the presence of the interstitial sink/source.

Figure 3: Example 18 - Silicon implanted into GaAs with the "plus one" interstitials created.

Figure 2: Corrected plot of Example 10 from Manual - GaAs MESFET Gate Simulation: Beryllium, Silicon, and Carbon profiles under the MESFET gate.

9 Figures

Figure 1: Corrected plot of Example 9 from Manual - Stress Dependent Oxidation: Comparison of LOCOS Shapes with 500Å Nitride and 1500Å Nitride.

[10] R.W. Jansen, D.S. Wolde-Kidane, and O.F. Sankey, "Energetics and Deep Levels of Interstitial Defects in the Compound Semiconductors GaAs, AlAs, ZnSe, and ZnTe," *J. Appl. Phys.*, **64**, 2415 (1988).

recent experimentation and calibration. In order to model various anomalous diffusion phenomena, the more advanced diffusion simulation models (Two.dim and Full.coupled) must be used. If the user wishes to use these modes, we have included the necessary GaAs defect parameters, based on theoretical work and on our own simulations of those phenomena. Finally we have given examples demonstrating the use of the new features as well as the use of Two.dim and Full.coupled diffusion modes in which anomalous diffusion behavior in GaAs is simulated. While most of the enhancements were added to improve GaAs process modeling, the new features and modeling techniques can also be used for silicon modeling.

8 References

References

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[8] W. Shockley and J.T. Last, "Statistics of the Charge Distribution for a Localized Flaw in a Semiconductor," *Phys. Rev.*, **107**, 392 (1957).

[9] G.A. Baraff and M. Schluter, "Electronic Structure, Total Energies, and Abundances of the Elementary Point Defects in GaAs," *Phys. Rev. Lett.*, **55**, 1327 (1985).

```
deposit nitride thick=.08
method fermi init=1e-2
diffuse time=0.001 temp=700
select z=log10(beryllium)
plot.1d x.min=-2 x.ma=1 y.mi=15.0 y.max=20.0
select z=log10((inter/ci.star)*1e17)
plot.1d cle=f axi=f line.type=5
method full.cpl init=1e-3
diffuse time=360 temp=700 argon
select z=log10(beryllium)
plot.1d cle=f axi=f
select z=log10((inter/ci.star)*1e17)
plot.1d cle=f axi=f line.type=2
quit
```

The deposit commands create the box-shaped Be doping regions. The method-fermi command and the initial diffuse step set the defects initially at their equilibrium concentrations. The method-full.cpl and 720 minute diffuse step then simulate the anneal with the dopant-defect interactions.

Figure 6 shows the Be profiles before and after a 12 hour anneal. Also shown are the corresponding C_I/C_I^* profiles. One can see that the Be profile develops kinks and shoulders in each side of the profile. This is a result of the interstitials pairing up with Be atoms in the high Be concentration regions causing a reduction in the local interstitial concentration, and unpairing in the low Be concentration regions (i.e. just ahead of the Be diffusion front) causing a supersaturation of interstitials there. The Full.coupled mode in SUPREM-IV.GS takes this into account and the C_I/C_I^* profiles show this. The resulting Be diffusion as simulated matches the actual data almost perfectly.

If one increases the anneal temperature to 900°C and then does the same simulation leaving all the other parameter expressions the same, the diffused Be profile will show the normal (equilibrium) box-shaped diffusion behavior. This is because the activation energies of the defect and dopant diffusivities are such that at the higher temperatures, the interstitial is fast enough relative to the Be diffusion so that nearly flat, equilibrium profiles of C_I/C_I^* are maintained.

7 Summary

Version 9450 of SUPREM-IV.GS, has been released. This version contains many enhancements to our gallium arsenide and silicon process simulator. New features were added, including defect sinks, and "plus one" defect creation. We fixed several bugs in the simulator. We decided to keep the dual set of GaAs diffusion models and parameters (for implanted versus grown-in dopants) as the default models, which can be quickly run using the Fermi diffusion method. Some of these parameters have been slightly modified for GaAs, based on

case, such as in high temperature grown-in Be (non-implanted) cases.

The actual experimental results for this, in terms of Be SIMS profiles, show excellent agreement to the SUPREM-IV.GS simulations for both short and long time anneals. The Two.dim diffusion mode is used rather than the Full.coupled mode, which is used in the next example, because the excellent fits to the experimental data. If the Full.coupled mode is used, an extra dip in the C_I/C_I^* profile occurs, due to the pairing of the dopant with the interstitials, and a kink in the Be profile results. The justification for not using this is that the dislocations that form (and are the basis for the sink used) can act as interstitial sources later on, and negate the effect of the pairing of interstitial and dopant. However, the sources must maintain a higher interstitial concentration than the equilibrium level in order to maintain the enhanced Be diffusivity, which the dislocations may indeed do. Using Two.dim with only the surface region sinks simplifies the simulation.

6.5.2 Example 21. Low Temperature Diffusion of Grown-in Be in GaAs using the Full.coupled Mode

In this example, the Full.coupled mode for diffusion is used to model the unusual behavior of high concentration grown-in Be in GaAs when annealed at low temperatures (700°C in this example). A box-shaped profile of Be in GaAs is used as the initial structure. No excess interstitials or vacancies are introduced - they are assumed to be at their equilibrium levels initially. However, the Full.coupled mode is used which allows for the pairing of dopants and defects, which is how the dopants is believed to diffuse (or via the kick-out, which results in the same effect). This results in local non-equilibrium of defects which can then affect the dopant diffusion. As in the previous example, the new values for the defect parameters are used here. Also, the same Be diffusivity is used as in the implanted example.

```
option quiet
set echo
mode one.dim
line x loc=0.0 spacing=0.04 tag=top
line x loc=3.5 spacing=0.04
line x loc=4.0 spacing=0.1
line x loc=80.0 spacing=10.0 tag=bottom
region gaas xlo=top xhi=bottom
boundary exposed xlo=top xhi=top
boundary backside xlo=bottom xhi=bottom
init beryllium conc=1e13
beryllium gaas Dix.0=0.0 Dix.E=0 Dip.0=0 Dip.E=0 Fi=1.0
beryllium gaas Dipp.0=0.17 Dipp.E=3.39 Fi=1.0
method inter rel.err=.1
method vacan rel.err=.1
deposit gaas thick=1 div=20 beryllium conc=1e19
deposit gaas thick=1 div=20 beryllium conc=1e13
```

```
interstitial gaas local.alpha=8.5e-1 dam.center=3.0e-5 dam.width=3.0e-5
diffuse time=2 temp=700 argon continue
select z=log10(beryllium)
plot.1d cle=f axi=f line.type=4
select z=log10((inter/ci.star)*1e15)
plot.1d cle=f axi=f line.type=2
quit
```

After the grid is set up and the initialization is done, a short (0.01 minute) Fermi diffuse step is done. This is to initially set the defect concentrations at their equilibrium levels for the upcoming anneal. (If this were done after the implant and "plus one" creation, the concentration of the interstitials in the bulk away from the implant would be nominally 0 and not the equilibrium value for the anneal temperature.) Using the plus.one option in the implant step, the interstitials (assumed to be Ga interstitials) are created identical to the implanted Be profile. After the initial profiles are plotted, the diffusion method is then switched to Two.dim, and the beryllium diffusivity is changed, as discussed above and in section 5. For these simulations, the Be is assumed to be electrically active only up to $2 \times 10^{17}\text{cm}^{-3}$ for the first two minutes. The act.a and act.b statements in the material command is used for this. Interstitial sinks/sources are created in an interstitial statement. The after-anneal dopant and defect profiles are then plotted.

Figure 5 shows the simulation results. Shown are the initial and final Be profiles. Also shown are the profiles of C_I/C_I^*, before and after anneal. (C_I^* is a function of doping concentration so that the initial C_I/C_I^* profile is different from the initial C_I and Be profiles.) The excess interstitials created by the "plus one" model increase the Be diffusion. The sink pulls the interstitial concentration down towards the surface, creating a gradient in C_I/C_I^* in the same direction. This causes anomalous diffusion in the tail region of the Be profile, creating an asymmetric kink in the profile. The gradient in the interstitials also causes Be diffusion towards the surface near the peak of the profile, resulting in "uphill diffusion" - uphill because the gradient in interstitials causes the Be to diffuse from a region of lower Be concentration to a region of higher Be concentration near the peak area.

For anneal times greater than two minutes, Hu [4] found that the the electrical activity of Be in GaAs should be reset to its default (and high) value. In addition, the sink/source for interstitials is removed. These are done by the commands:

```
material gaas p.type act.a=1.0 act.b=1e21
interstitial gaas local.alpha=0 dam.center=0 dam.width=0
```

following the 2 minute anneal. Then the diffuse step, with the continue option, is done for the remainder of the anneal.

If the diffuse time is increased to 30 minutes (not shown), it can be seen that the C_I/C_I^* profile becomes close to flat, yet still above the value of unity (unity would mean that the $C_I = C_I^*$ and that interstitials are at their equilibrium value). The flat C_I/C_I^* profile results in the Be profile becoming the normal box-shaped profile again, while the higher-than-one C_I/C_I^* value means that the effective diffusivity of Be will still be greater than the equilibrium

based on work by Hu *et al.* [4, 5, 6]. They make use of two of the new features in SUPREM-IV.GS: the "plus one" defect creation model for implantation; and the interstitial sink (see Examples 18 and 19), as well as the new dopant and defect parameters (see section 5). By using these and the more advanced diffusion modes (Two.dim and Full.coupled), the diffusion of both implanted Be and grown-in Be can be modeled with the same parameters for Be diffusivity, and we can accurately model much of the anomalous diffusion behavior in GaAs.

6.5.1 Example 20. Tail and Uphill Diffusion of Implanted Be in GaAs using Two.dim Mode

In this example Be is implanted into GaAs and annealed for a short time. The "plus one" model is used to produce excess interstitials (so that the initial excess interstitial profile equals the implanted Be profile), and an independent interstitial sink is used from the surface to a depth of 0.6 microns. The sink is presumably due to dislocations formed by the implant and anneal. The defect parameters used are the new numbers (see section 5). The beryllium diffusivity values are those which should be used only when using either the Two.dim or Full.coupled modes. (The default numbers, which are different, are to be used when the Fermi method is used.) The Two.dim mode is used for the diffuse step.

```
option quiet
set echo
mode one.dim
line x loc=0.0 spacing=0.02 tag=top
line x loc=1.5 spacing=0.05
line x loc=80.0 spacing=10.0 tag=bottom
region gaas xlo=top xhi=bottom
boundary exposed xlo=top xhi=top
boundary backside xlo=bottom xhi=bottom
init beryllium conc=1.5e10
method inter rel.err=.1
method vacan rel.err=.1
method fermi init=1e-3
diffuse temp=700 time=0.01
implant beryllium dose=1e14 energy=150 pearson plus.one
deposit nitride thick=.08
select z=log10(beryllium)
plot.1d x.min=0.0 x.max=2.0 y.mi=15.0 y.max=22.0
select z=log10((inter/ci.star)*1e15)
plot.1d cle=f axi=f line.type=2
method Two.dim init=1e-3
beryllium gaas Dix.0=0.0 Dix.E=0 Dip.0=0 Dip.E=0 Fi=1.0
beryllium gaas Dipp.0=0.17 Dipp.E=3.39 Fi=1.0
material gaas p.type act.a=1.0 act.b=2e17
```

Figure 4 shows the interstitial profile before and after anneal. The initial interstitial profile is the same as the implanted silicon profile (not plotted), while the post-anneal interstitial profile shows the effect of the independent sink/source. The interstitial concentration is pulled down towards the equilibrium interstitial concentration ($1 \times 10^{15}\text{cm}^{-3}$ in this example) in the region of the sink/source.

```
option quiet
set echo
mode one.dim
line x loc=0.0 spacing=0.02 tag=top
line x loc=0.5 spacing=0.02
line x loc=20 spacing=0.25 tag=bottom
region gaas xlo=top xhi=bottom
boundary exposed xlo=top xhi=top
boundary backside xlo=bottom xhi=bottom
init
interstitial gaas D.0=5e-14 D.E= 0.
interstitial gaas Kr.0=0 Kr.E= 0.
interstitial gaas Cstar.0= 1.0e15 Cstar.E= 0.
interstitial gaas /gas Ksurf.0= 0 Ksurf.E= 0.
interstitial gaas neu.0=1 neu.E=0 pos.0=0 pos.E=0 dpos.0=0 dpos.E=0
interstitial gaas tpos.0=0 tpos.E=0 neg.0=0 neg.E=0 dneg.0=0 dneg.E=0
interstitial gaas tneg.0=0 tneg.E=0
interstitial gaas local.alpha=8.5e-1 dam.center=3.0e-5 dam.width=1.0e-5
implant isilicon dose=5e13 energy=150 pearson plus.one
select z=log10(interstitial)
plot.1d x.min=0.0 x.ma=1.5 y.mi=14.0 y.max=20.0 line.type=1
method Two.dim init=1e-5
diffuse time=2 temp=700 argon
select z=log10(interstitial)
plot.1d cle=f axi=f line.type=2
quit
```

The sink/source can be changed or removed at any point in the simulation by adding a new interstitial statement with new sink/source parameters (equal to zero to remove it).

6.5 Examples Showing the Use of Two.dim and Full.coupled Diffusion Modes for Anomalous Be Diffusion

In these examples, Two.dim and Full.coupled diffusion modes are used to simulate some anomalous behavior of implanted and grown-in beryllium in GaAs, respectively. They are

6.4.1 Example 18. The "Plus one" interstitials defects

In this example we show how one can simulate the "plus one" interstitial defects created by the implantation of a dopant. Silicon is implanted into GaAs and the "plus one" interstitial defects are created by using the plus.one option in the implant command. In Figure 3 the created interstitials are shown. The dopant (silicon) profile would be identical.

```
option quiet
set echo
mode one.dim
line x loc=0.0 spacing=0.02 tag=top
line x loc=0.5 spacing=0.02
line x loc=20 spacing=0.25 tag=bottom
region gaas xlo=top xhi=bottom
boundary exposed xlo=top xhi=top
boundary backside xlo=bottom xhi=bottom
init
implant isilicon dose=1e13 energy=150 pearson plus.one
select z=log10(interstitial)
plot.1d x.min=0.0 x.ma=1.5 y.mi=14.0 y.max=20.0 line.type=1
quit
```

Note: if you want the interstitial profile to equal the equilibrium interstitial profile beyond (deeper than) the implanted profile, then a negligible-time Fermi diffuse step should be done at the appropriate temperature before the implant step. The "plus one" interstitials will then be added on to the equilibrium interstitials. (If the Fermi diffuse step is done *after* the implant step, the "plus one" defects will be erased.)

6.4.2 Example 19. Point Defect Sink and Source

In this example, an interstitial sink/source is created which independently brings the interstitial concentration in that region closer to equilibrium (i.e. independent of vacancies). The independent interstitials sink/source is created in an interstitial statement:

```
interstitial gaas local.alpha=8.5e-1 dam.center=3.0e-5 dam.width=1.0e-5
```

which places the sink/source at a location of 0.2 to 0.4 microns from the surface (*i.e.* centered at 0.3 microns from the surface with a width of 0.1 microns on either side of the center, or a total width of 0.2 microns), with a strength of 0.85 (arbitrary units). Non-equilibrium interstitials are created by implanting silicon into GaAs and using the plus.one interstitial option in the implant command (see previous example). The GaAs is then annealed, using the Two.dim method and diffuse statements. In the interstitial command lines, the bulk (I-V) recombination and surface recombination are set to zero, and for simplicity only neutral interstitials are considered. Also, arbitrary values are used for the interstitial diffusivity and equilibrium concentration.

given, with both the input files and output plots. These serve to illustrate the use of some of the new features discussed above, as well as to demonstrate how more advanced, optional models can be used to simulate more complex GaAs behavior.

6.1 Corrected Example 9 Figures in 1993 Manual

The figure for "Example 9: Stress Dependent Oxidation" in the Manual, had showed the incorrect graphical representation. Figure 1 in this addendum shows the correct representation.

6.2 Corrected Example 10 Figure in 1993 Manual

The figure for "Example 10: GaAs MESFET Gate Simulation" in the Manual contained an error. The Si profile shown was incorrect. The corrected simulation is shown in Figure 2.

6.3 Comment on Example 16 in 1993 Manual

"Example 16: Two.dim Diffusion with File Input Interstitials" in the Manual illustrated a simulation using the Two.dim method, using old, rather arbitrary defect parameters. An initial Fermi method diffuse step probably should have been used to set up the initial conditions for the defect parameters, specifically the interstitial and vacancy concentrations. This is apparent if one runs this example using the new version 9450 code: one gets a different result compared to when running the 9305 code. (Note: all other examples in the original manual will give the same result using either code.)

The reason for this difference is that for the Two.dim and Full.coupled methods, the initial defect parameter values are first set in the "init" step. It arbitrarily sets them to their 900°C values. If these are not specified in the input file *before* this command, then the modelrc values are used. Since the modelrc values are different for the two versions of SUPREM-IV.GS for these, then different simulation results occur.

To get the example to give the same results as before, one can simply add the following statements immediately before the "init" statement:

interstitial gaas Cstar.0= 1.0e14 Cstar.E= 0.

vacancy gaas Cstar.0= 1.0e14 Cstar.E= 0.

This sets the initial defect concentrations to the same values that the 9305 modelrc file does, and the same profiles can now be obtained as shown in the figures in the manual. As mentioned above, a short Fermi diffuse step before the Two.dim diffuse step should bee done (as shown in Example 17). This (re)sets the initial defect parameters at the temperature you wish, and removes any ambiguity.

6.4 Examples Showing the Use of New Features

The following examples in GaAs demonstrate the use of some of the new features in SUPREM-IV.GS. (The examples are numbered to follow the examples given in the original manual.)

Schluter [9] and Jansen *et al.* [10]. The latter had determined that the Ga interstitial surrounded by Ga atoms has a lower energy of formation than the Ga interstitial surrounded by As atoms. Baraff and Schluter [9] calculated that for this species the 1+ charge state is the equilibrium state throughout the band gap. We previously calculated its probability assuming that its energy level is right at the conduction band edge at all temperatures, even though its energy level may be anywhere at or above the conduction band edge. This led to a finite probability of neutral Ga interstitials. This time we assume that the 1+ Ga interstitial is the only interstitial present in GaAs for all temperatures (i.e. its relative probability is unity). This is based both on successful simulations of Be diffusion in GaAs [4], and also the acknowledgement that the 1+ charge state energy level may be anywhere above the conduction band edge, and that it being right at the conduction band edge is very unlikely. At worst, this change can only make a two times difference in the total interstitial concentration for the highest n-type doping conditions as compared to the previous numbers.

The new default values are:

```
interst gaas neu.0=0 pos.0=1 neg.0=0 dneg.0=0 dpos.0=0
interst gaas neu.E=0 pos.E=0 neg.E=0 dneg.E=0 dpos.E=0
interst gaas tpos.0=0 tpos.E=0 tneg.0=0 tneg.E=0
vacancy gaas neu.0=1 pos.0=0 neg.0=18.214 dneg.0=330.21 dpos.0=0
vacancy gaas neu.E=0 pos.E=0 neg.E=-0.56 dneg.E=-0.8 dpos.E=0
vacancy gaas tneg.0=5591.8 tneg.E=-0.81 tpos.0=0 tpos.E=0
```

Hu [4, 5, 6] found in his simulations of Be diffusion in GaAs, using the Two.dim or Full.coupled modes, he could best model the diffusion of beryllium (both implanted and grown-in) by using a diffusivity proportional to p^2, where p is the local hole concentration, as opposed to p, which was originally used in the default implanted/grown-in diffusivities. (As discussed above, the default grown-in Be diffusivity as now been changed to a p^2 term.) The values used in his simulations for both implanted and grown-in are:

```
beryllium GaAs Dipp.0= 1.7e-1 Dipp.E= 3.39
```

and all other Be diffusivity values equaling 0. This should only be used when using Two.dim or Full.coupled and the initial defect conditions ("plus one" interstitials, etc.). When using the Fermi method, one should use the default diffusivities for best overall fits - these are:

```
beryllium gaas Dip.0 = 0 Dip.E = 0 Dipp.0=3.19e3 Dipp.E= 4.41 grown.in
beryllium gaas Dip.0 = 2.1e-6 Dip.E = 1.74 Dipp.0 = 0 Dipp.E = 0 implanted
```

6 Examples

First, some comments and corrections to the examples in the original 1993 SUPREM-IV.GS Manual are given. Then several examples of SUPREM-IV.GS - version 9450 simulations are

to dump the one dimensional profile data (as a series of depth-concentration pairs) to a new file.

5 Parameters Added for Two.dim and Full.coupled Diffusion Modes

As mentioned earlier, using the more advanced point-defect diffusion methods (or modes) in SUPREM-IV.GS (Two.dim and Full.coupled), as opposed to the default mode (Fermi), some of the anomalous diffusion behavior in GaAs can be accurately simulated. By using these one can even eliminate the use of dual diffusivities (implanted versus grown-in) and use the same values for both cases, and thus use more "physically-correct" models. To do so one must have values for a number of defect parameters. In addition, the dopant parameters may have to be changed, as is the case for beryllium diffusion - the only dopant so far extensively calibrated for Two.dim and Full.coupled simulation.

The following GaAs parameter values have been determined by Hu *et al.* [4, 5, 6] mostly based on experiments, SIMS analysis, and SUPREM-IV.GS fitting of Be diffusion in GaAs. The determination of the (gallium) vacancy equilibrium concentration (Cstar) and diffusivity are based on reference [7].

```
interst gaas D.0=6.4e-5 D.E=1.28
interst gaas Kr.0=6.2e-11 Kr.E=1.31
interst gaas Cstar.0=4.7e28 Cstar.E=3.25
interst gaas /nitride Ksurf.0=1e-4 Ksurf.E=0 Krat.0=0 Krat.E=0
interst gaas /nitride Kpow.0=1 Kpow.E=0
vacancy gaas D.0=3.9e-4 D.E=1.7
vacancy gaas Kr.0=6.2e-11 Kr.E=1.31
vacancy gaas Cstar.0=8.17e35 Cstar.E=4.26
vacancy gaas /nitride Ksurf.0=1e-4 Ksurf.E=0 Krat.0=0 Krat.E=0
vacancy gaas /nitride Kpow.0=1 Kpow.E=0
```

The above numbers will be the default values for these parameters in this version of SUPREM-IV.GS since these parameters will be used only when the Two.dim and Full.coupled methods are used.

The values of the defect energy levels in GaAs were also recalculated since the last version. For the vacancies we again calculated the relative probability of each charge state using the Shockley-Last equations [8], using the energy levels of the variously charged vacancies calculated by Baraff and Schluter [9]. The relative probability of each charge state was calculated using the Shockley-Last equations [8]. However this time we assumed the defect energy level follows the conduction band edge as the temperature changes, as opposed to following the valence band edge.

For the interstitials we base the energy levels on the theoretical work of Baraff and

A couple of modifications have been made to the default GaAs diffusion parameters in the current version. First, the diffusivity for grown-in Be has been changed to:

beryllium gaas Dip.0 = 0 Dip.E = 0 Dipp.0=3.19e3 Dipp.E= 4.41 grown.in

based on recent analysis of our data. The hole dependence is thereby changed from linear to quadratic, which better fits the shape of the profiles as well as the extent of diffusion when one changes the peak concentration. (The hole dependence of implanted Be diffusivities in the default/Fermi mode will remain linear, with Dip.0=2.1e-6, Dip.E=1.74, Dipp.0=0, and Dipp.E=0, since the extent of diffusion for different doses is best fit by this linear dependence.) Secondly, the diffusivities for implanted Zn have been modified. The previous implanted Zn diffusivity was based on two sets of experimental data, both obtained at Stanford; an average of the two sets at each temperature was used as the default number. However, recent results agree with the earlier set and therefore we are now using only those numbers. The latter set may have been affected by failure of the nitride cap. The new numbers for implanted Zn diffusion are now:

zinc gaas Dipp.0 = 3.9e-3 Dipp.E = 2.73 implanted

4 Other Changes

4.1 Expressions for Dopant Activation

In the first manual, values for the dopant activation model for n and p type dopants were incorrectly given in Example 12: "Dopant Activation Model." The commands and correct default numbers for GaAs are:

material gaas p.type act.a="(1)" act.b="1.00e21"
material gaas n.type act.a="(2.2 - 0.00117 * T)" act.b="1.25e18"

The example showed what happens when act.b for the n.type dopant is changed from 1.25e18 to 4.25e18.

4.2 Creating Output File for Export

Often one would like to plot the SUPREM results using a different program or application. The output file using the structure.out command is not usually useful for this. However, one can use the print.1d command. After a variable is selected using the select command, one can use:

print.1d > "filename"

where $rect(y)$ is the unit gate function given by:

$$rect(x) = \begin{cases} 1 & \text{for } |x| < 0.5 \\ 0 & otherwise \end{cases} \tag{5}$$

and y_0 is the center of a localized source/sink, W is the width of such a source/sink and α_G and α_L are, respectively, the efficiencies of the global and the local source/sink. In SUPREM-IV.GS, the dimensions are specified in cm and the efficiencies in sec^{-1}. It should be noted that the $\varphi_I^{(s)}$ act interchangeably as sources and as sinks according to whether the interstitial concentration is, respectively, less or more than the equilibrium value. A similar model is also implemented for vacancies.

The source/sink model can be used in SUPREM-IV.GS for either GaAs or Si by using the interstitial or vacancy commands and the following options:

[glob.alpha=< n >]
[local.alpha=< n >]
[dam.center=< n >]
[dam.width=< n >]

in which glob.alpha corresponds to α_G in equation 4 above, local.alpha corresponds to α_L, dam.center corresponds to y_0, and dam.width corresponds to W. For example:

interstitial gaas local.alpha=8.5e-1 dam.center=3.0e-5 dam.width=1.0e-5

places an interstitial sink/source at a location of 0.2 to 0.4 microns from the surface (*i.e.* centered at 0.3 microns from the surface with a width of 0.1 microns on either side of the center, or a total width of 0.2 microns), with a strength of 0.85 (arbitrary units). The command:

interstitial gaas glob.alpha=8.5e-1

places an interstitial sink/source throughout the GaAs with a strength of 0.85.

This has been utilized by Hu, *et al.* [4, 5] to model uphill and tail diffusion of implanted Be in GaAs.

3 Default Diffusion Models and Parameters

In the initial version of SUPREM-IV.GS, the default diffusion method or mode for GaAs was the Fermi method. For the default diffusion parameters, two sets of diffusivities for the eight GaAs dopants were used: one for when the dopant was implanted, and one for when the dopant was grown-in. These differences are believed to be due to different point defect conditions caused by the introduction of the dopants and the subsequent diffusion. For simulation running time considerations, as well as for simplicity, these remain the default models in the current version.

terstitials were already present. Note that this adds the "plus one" profile to the existing interstitial concentration, it does not wipe out the previous numbers. For example, if you had previously done a Fermi diffuse step to set the interstitials at some temperature-dependent equilibrium level, the plus.one option in the implant statement would add the "plus one" interstitials to that level at each position.

2.2 Point Defect Sinks and Sources

Another new feature added to SUPREM-IV.GS is the ability to model point defect sinks or sources. This is very similar to recombination of interstitials or vacancies at the surface (using the Ksurf parameter), except that this reduction or generation of point defects can now occur over a finite length anywhere in the bulk. This could be due to the annihilation or generation of the point defects at dislocations.

The previous model for interstitials can be expressed as:

$$\frac{\partial \left(C_I - C_{ET}\right)}{\partial t} = \nabla \left(-J_I - \sum_{imp} J_{AI} \right) - R \tag{1}$$

where C_I is the interstitial concentration, C_{ET} is the empty trap concentration, J_I is the interstitial flux, J_{AI} is the diffusing impurity flux and R is the bulk recombination. (An analogous model involved vacancies.) A boundary condition on the interstitials allows for injection and/or recombination at the surface.

In some situations there is a need to simulate interstitial sources or sinks which act to return the concentration of interstitials to its equilibrium value. The formation of dislocation loops in a semiconducting substrate as a result of implant damage is an example of such a phenomenon. It is also desirable that we have the ability to specify such sources/sinks either throughout the bulk or in a localized manner. In other words, we wish to expand (1) to:

$$\frac{\partial \left(C_I - C_{ET}\right)}{\partial t} = \nabla \left(-J_I - \sum_{imp} J_{AI} \right) - R + \varphi_I^{(s)}(y) \tag{2}$$

where y is the depth into the wafer.

$\varphi_I^{(s)}$ is different from R since the latter must involve vacancies as well as interstitials:

$$R = K_R \left(C_I C_V - C_I^* C_V^* \right) \tag{3}$$

where the superscript * refers to equilibrium concentrations. The sources and sinks also cannot be easily modeled using the trap reaction in that it changes the concentration of empty traps, thereby making the source/sink efficiency a time-dependent quantity.

We have implemented a mechanism with the desired features in SUPREM- IV.GS with the expression:

$$\varphi_I^{(s)}(y) = \left(\alpha_G + \alpha_L \cdot rect\left(\frac{y - y_0}{W} \right) \right) \cdot \left(C_I - C_I^* \right) \tag{4}$$

Much of the anomalous diffusion behavior of dopants in GaAs can be modeled in SUPREM-IV.GS by using the point defect based diffusion models (i.e. Two.dim and Full.coupled). This anomalous behavior includes uphill and tail diffusion after implantation, kinks in the diffusion profiles for grown-in dopants, and even the difference between the effective diffusivities of dopants that were implanted and that were grown-in. Even though the simple Fermi method models and parameters are the default models - mostly for simulation time considerations, one may use more advanced models to simulate these phenomena. To assist one in this we present in this addendum our latest determinations of various point defect parameter values for GaAs, as well as give examples of modeling the diffusion of implanted and grown-in Be in GaAs using these models and parameters.

Most of the new features have been added as a result of research and modeling of GaAs technology. However, any of these features may be used for silicon modeling as well. We believe that modeling many of the "anomalous" effects in silicon might also be aided by using these new features.

2 New Features Added

The new version of SUPREM-IV.GS includes some new features, which will be discussed below. Examples of using some of these in GaAs are at the end of this addendum.

2.1 Implant Induced Defects

When implanting dopants into a semiconductor material, point defects are generated. These are of three types: (1) Frenkel pairs of equal numbers of interstitials and vacancies; (2) vacancies at the surface due to sputtering of substrate (target) atoms; and (3) interstitials equal in total number to the incoming ion dose due to the ions eventually all becoming substitutional (called the "plus one" model). If it is assumed that during annealing all Frenkel pairs recombine, and that the vacancies due to sputtering are confined to the surface [1], then the interstitials created by dopants becoming substitutional may become the dominate point defects. Giles [2] proposed that the "plus one" defects do in fact dominate the transient diffusion of implanted phosphorus in silicon, and Griffin *et al.* [3] use this to model implanted boron diffusion in silicon. In addition, Hu, *et al.* [4, 5] use this to model the transient tail and uphill diffusion of implanted Be in GaAs. The modeling of this is simple: a profile of interstitials is created identical to the implanted dopant profile. This assumes that the dopant becomes interstitial before any significant diffusion of the dopant occurs.

This "plus one" model for interstitial defects created during implantation has been added to SUPREM-IV.GS for both GaAs and Si. To use it, add the option [plus.one] to the implant statement. For example:

```
implant isilicon dose=1e13 energy=150 pearson plus.one
```

This will add an interstitial profile equal to the implanted dopant profile to whatever in-

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Addendum to Manual: SUPREM-IV.GS – Two Dimensional Process Simulation for Gallium Arsenide and Silicon

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(Note: You will notice that the actual figures are currently missing from the online version of this addendum. We are working on reformatting this document to include all the figures referenced.)

1 Introduction

In 1993 SUPREM-IV.GS was first released. This was the first version of SUPREM-IV which models GaAs and it dopants in addition to modeling silicon technology. In the initial version of SUPREM-IV.GS, GaAs models and parameters developed previously for SUPREM 3.5, a 1D GaAs-only process simulator, had been added to SUPREM-IV, a 2D point-defect based Si process simulator. Since then we have enhanced SUPREM-IV.GS for GaAs by adding new features, modifying some parameter values, and including GaAs point defect parameters necessary to utilize SUPREM-IV's advanced diffusion models. The latest release of SUPREM-IV.GS, version 9450, is presented and discussed in this addendum.

Several new features have been added to SUPREM-IV.GS. Implant induced defects, in terms of interstitials created when implanted dopants become substitutional, can now be included in the implant simulation. Also added are point defect sinks and sources which can extend over a user-defined area in the semiconductor. Each of these new features will be discussed, and the parameter names and algorithm equations will be given. Examples of using these for GaAs will be shown.

The default models for diffusion in GaAs - using the "Fermi" diffusion method or mode and having separate parameters for implanted dopants and grown-in dopants - have remained the same. A few of the parameter values have been modified based on recent experimental results and modeling, and these will be listed.