

Electrical Calculations for Suprem4

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Abstract

Suprem4 lacks built in facilities for modeling electrical parameters. Using Suprem4's shell script facilities this can be overcome by linking Suprem4 with Suprem3, which does have electrical modeling capabilities. This paper describes a Suprem4 macro file that provides electrical calculations for Suprem4 with minimal complexity for the end user.

1 Introduction

Feature sizes in advanced semiconductor technologies are driving the move from one dimensional simulation to two dimensions. Within National, the two dimensional simulator of choice is Suprem4 from TMA.

In addition to it's two dimensional representation, Suprem4 incorporates many advanced physical models, such as those for the diffusion of interstitials and vacancies, and stress models. However it's output tends to limit it's use to more sophisticated users. The only two current output methods are via the plot statements, and the print.lid statement. If the user wants data these two commands cannot offer, they are forced to link the structure to other tools such as Medici, or run separate Suprem3 simulations.

Suprem4's predecessor, Suprem3, still has several features that are not yet found in Suprem4. Examples of this includes the electrical, and extract statements.

In this paper we discuss the creation of Suprem4 macro files to greatly enhance the users capabilities, with a minimum of additional complications.

Suprem4 and Suprem3 commands are shown in **courier bold** in the following discussion. Unix commands are shown in *courier italic*.

2 Macro Use

The section covers the use of the macro, details of it's operation are in the next section. Macro use simply requires the user to add four lines to their input file, wherever an electrical result is required. An example of the lines from a file are:

```
define ElectTemp 1000  
  
define ElectX      1.0  
define ElectDepth  2.0  
source S4Electric.s4in
```

The ElectTemp define stores a temperature value to be used in calculating solid solubilities. The next define, ElectX, is used to select the x coordinate at which the 1D slice is taken, this may be anywhere within the limits of the users structure. The final define, ElectDepth, stores the maximum depth from which electrical results are extracted. ElectDepth is particularly useful for limiting the electrical calculation to the region of actual interest when using very deep simulation structures such as those required by the **TWO.DIM** model. All three defines are required, although once the values are stored, multiple calls to the macro may be made with out redoing the defines. The source statement runs the macro.

3 Principles of Operation

The shell command facility of Suprem4 offers the ability to link with virtually any other tools on the UNIX network. The shell command is invoked with the ! symbol. For example the following command

```
! ls
```

will cause Suprem4 to issue the system ls command to list the files in the current directory. The UNIX *echo*

command can be combined with the Suprem4 shell command to write information to specific files. For example

```
! echo      line number 1> a.file
! echo      line number 2>> a.file
```

creates a two line file called a.file.

Using this simple feature the s4electric macro file performs six steps necessary to link to Suprem3 and generate results. In order of execution, the steps are initialization, data extraction, Suprem3 data import, calculation, parsing, and cleanup.

3.1 Initialization

The initialization portion of the macro pre-defines several variables that make the macro file simple to move between systems. These define calls to awk, Suprem4, and Suprem3. The Suprem4 define also sets up a temporary output file name so the current output file is not overwritten. The initialization block next saves the current structure, and writes a short awk program, the function of which will be discussed further below.

3.2 Data Extraction

The extraction consists of six lines of code, that are repeated 4 times, once for arsenic, boron, antimony, and phosphorus. The first three lines define a short Suprem4 input file whose structure is:

```
init file=Elect.Structure
select z=active(arsenic) +
      temp=@{ElectTemp}
print x.v=@{ElectX} +
      x.max=@{ElectDepth}
```

The temperature is included in the **select** command to insure that effects of any included rampdowns are negated.

The fourth line of the block runs the Suprem4 program, generating an output file containing 1D profile data for arsenic. The profile generated can not be read by Suprem3 yet. The fifth line of the block uses the UNIX **grep** command to extract the silicon doping information to a temporary file.

The silicon interface in Suprem4 need not have a depth value of zero, later use of the Suprem3 **PROFILE** statement however will require it. The final line of the block uses the previously defined awk program to zero the interface point.

As noted above this is repeated three more times to extract all four dopants. The only change required for each successive iteration is the dopant on the select statement. At the end of the data extraction we have four files containing the profile data.

3.3 Data Import

The next task is to get this information into Suprem3. Again the **! echo** construct is used. This time we write a Suprem3 file. This file is as follows:

```
initial Si Thick=@{ElectDepth} spac=950
profile arsen active      +
      file=Electrical.profile.Arsenic
profile phosp active     +
      file=Electrical.profile.Phosphor
profile antim active     +
      file=Electrical.profile.Antimon
profile boron active     +
      file=Electrical.profile.Boron
diffusion temp=1300 time=0.0001
```

The number of spaces is chosen to be large to be as general as possible in the structure. The Diffusion statement is used to set the temperature high enough to insure that all dopant passed to Suprem3 is active.

3.4 Calculation

Now we are ready to define the desired calculations, and execute them. The initial version of this program used only Suprem3's electrical calculation capabilities. This is the only case I will describe here, although the possibilities are limited only by Suprem3's capabilities. The zero bias electrical calculation is carried out by simply appending a **PRINT ELECTRICAL** statement to the Suprem3 input file, and executing Suprem3 with the file as input. The result is a Suprem3 output file containing the desired result.

3.5 Parsing

The electrical data has been successfully generated, however the current state is undesirable. The electrical output is in file separate from our Suprem4 output, with no apparent causal connection to the Suprem4 output. If we execute the electrical macro again from this Suprem4 simulation we will also lose the first run data. The parsing block solves this by extracting the results of the Suprem3 electrical statement, and putting it into the Suprem4 output file.

The Suprem3 electrical output begins at line 50 of the s3out file. The lines are extracted using the UNIX *sed* editor, and piped to *awk* where each line is pre-pended with a `$S4Elec;`, and saved to a temporary file. Next the Suprem4 macro issues a Suprem4 `source` command with the temporary file as input, which causes the data to be listed in the output file.

It is in the parsing stage that creativity is required as more Suprem3 calculations such as VT's, capacitance, SRP's or junction depths are added to the a macro. In the general case it is difficult to determine the relevent lines, so that they can be extracted and included in the output file. If the user has a specialized task, and structure to simulate, then it simply becomes a matter of counting lines in the Suprem3 output file. It is the generalized case that is difficult.

3.6 Cleanup

As a final step the macro uses a Suprem4 shell command to remove all temporary files created.

4 Results

Using simple simulations that insure that the physical models used by both Suprem3 and Suprem4 are similar, I have compared results and found them to be within 1-2%. It must be emphasized that comparisons are only valid if the same models are used in both Suprem3 and Suprem4, and the grid structure is sufficient in both. The technique has also been extended to the generation of SRP plots for correlation, however this module is not yet ready for general release.

5 Limitations

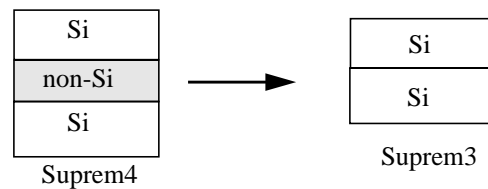
There are several limitations to this method, many of which can be overcome by the inclusion of a 1D electrical calculation directly into Suprem4.

Due to Suprem3 the electrical calculation is inherently 1D. It is crucial that the user selects a X position to such that contours of doping would be constant for a fixed Y depth. Data generated through curved regions can be interpreted, but it's reliability is unknown.

Suprem3 has a built in limitation to the electrical calculation. Suprem3 does the electrical calculation by calculating the conductance at each node, and adding the conductances within a diffusion region. Suprem3 prints the inverse as the sheet resistance. This ignores the vertical components normally present in a sheet resistance measurement. For many structures this is unimportant,

however for buried layers with a highly resistive epi layer, it may lead to a prediction that is lower than the measured sheet resistance. Simulations with Medici can be used to show that this is indeed the case.

Due to the nature of the method used to extract the data from Suprem4, it is imperative that there be only a single layer of silicon present. If more than one layer is present, the extraction will remove any non-silicon layers in the 1D slice, and pass the remains on to Suprem3 as a single piece of silicon. The following figure shows the effect graphically. This is only a minor limitation



since most simulations contain only a single layer of silicon. It is possible to overcome this by adding a minimum depth parameter for the profile extraction. This will not be discussed here.

Although Suprem3 now contains dynamic clustering models, Suprem4 does not. The use of a fixed temperature to set solid solubilities is a problem if more than one diffusion region exceeds solid solubility, and those regions have seen different thermal histories. This may force the user to set solid solubility for one or more regions either too high or too low, since only a single temperature setting is available.

6 Future Expansion

The currently released module contains only electrical calculations. A module to generate SRP data has been created, and tested, but the output needs to be cleaned up prior to release. Future modules are envisioned which perform 1D capacitance calculations, 1D VT calculations, and extract depletion region edges.

Beyond these it is possible to use other tools such as Medici, for calculations. For example of Medici could be used for an accurate calculation of sheet resistance (four point probe results) for deep buried layers, by including vertical resistance elements. This would be useful from Suprem3 also, but unfortunately Suprem3 is unable to execute shell commands.

7 Challenge to Reader

To conclude I offer a challenge to readers to create more Suprem4 macros that are general in nature, and to share them via the TCAD bulletin board. Specialized modules would also be appreciated since other users can adapt them to their needs.

The use of Suprem4's shell command capabilities provides an extremely powerful capability. The above example concerns itself with the linking of Suprem3. However, using the same feature it is possible to add in links to Depict, Medici, Minimos and others. The possibilities are very promising.