Process simulation

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Athena overview

Athena is a process simulator that provides general capabilities for numerical, ***physically-based***, two-dimensional simulation of processes used in semiconductor industry (ion implantation, diffusion, oxidation, physical etching and deposition, lithography,...).

Athena input file

- It is a ***text file*** that can be arranged by using Deckbuild or any text editor.
- It collects a sequence of commands (***statements***) corresponding to the individual steps of a process flow and control commands specified to select physical models and parameters.

Athena simulation

- Generating Athena ***input file***
- Running Athena ***simulation***
- Analyzing Athena ***output file***

Simulation problem specification

The simulation problem must be specified in the ***input file***, defining the following steps:

Initial geometry
Simulation grid *Initial substrate*
Sequence of process steps
Epitaxial growth *Layers deposition* *Geometrical etching* *Ion implantation* *Diffusion*
Physical models
Implant models *Diffusion models* *Oxidation models*

Running Athena simulation

Running Athena inside Deckbuild

To run Athena inside Deckbuild use the following command line:

> *go athena*

Running a given Athena version

The syntax is:

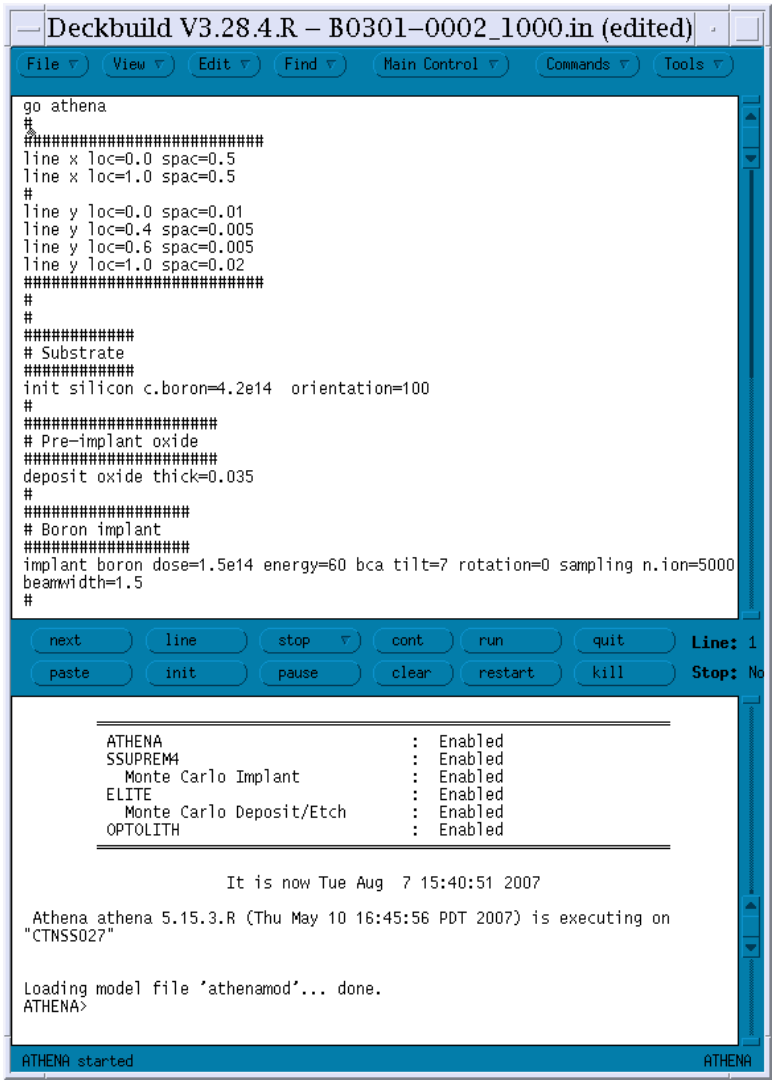
> *go athena simflags="-V 5.8.0.R"*

Running Athena without Deckbuild

To run Athena directly under unix use the following command line:

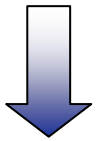
> *athena <input filename>*

> *athena –V 5.8.0.R <input filename>*



Athena output file

The main Athena output is the ***Standard Structure File***, a universal file format used by Silvaco simulation programs. The STRUCTURE statement of Athena creates a Standard Structure File (***.str***), which contains mesh and solution information, model information, and other related parameters.



The saved Structure File can be used by:

- ***Athena*** to continue process simulation
- ***Atlas*** or other device simulators to perform electrical analysis
- ***Tonyplot*** to graphically display the structure created by Athena
- ***Devedit*** to modify the mesh and the structure before running a device simulation

Question 1

A process simulation problem must be specified in the:

a) output file

b) input file

c) Standard Structure File

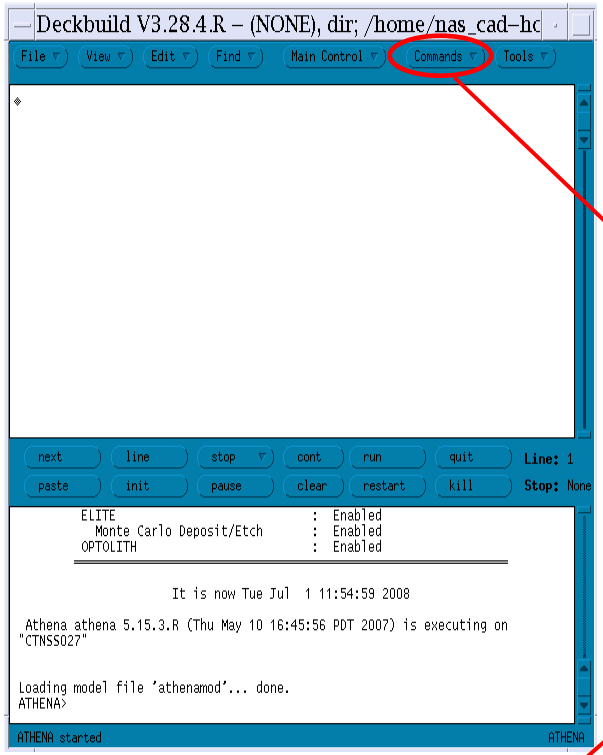
Creating a device structure

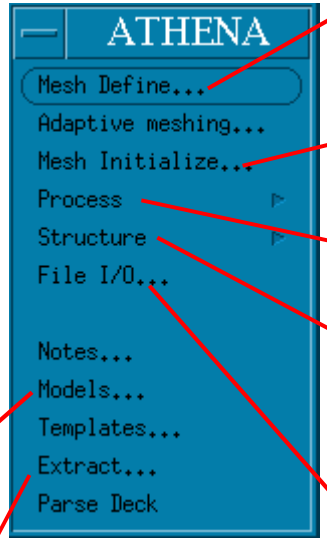
The following section will describe how to use Deckbuild interface in order to create a typical Athena ***input file***. In particular, the process simulation of a simple *pn* diode is described.

Basic *operations* to create the input file
Developing a good simulation ***grid***
Defining initial ***substrate***
Performing layer ***deposition***
Performing geometrical ***etching***
Performing ion ***implantation*** and ***diffusion***
Specifying the ***electrodes***
Saving the ***structure file***

Running Athena inside Deckbuild

The *Commands* menu includes the *statements* of the current simulator





To define simulation grid

To define initial substrate

To specify process steps

To specify electrodes

To save a structure file

To access Athena coefficients file

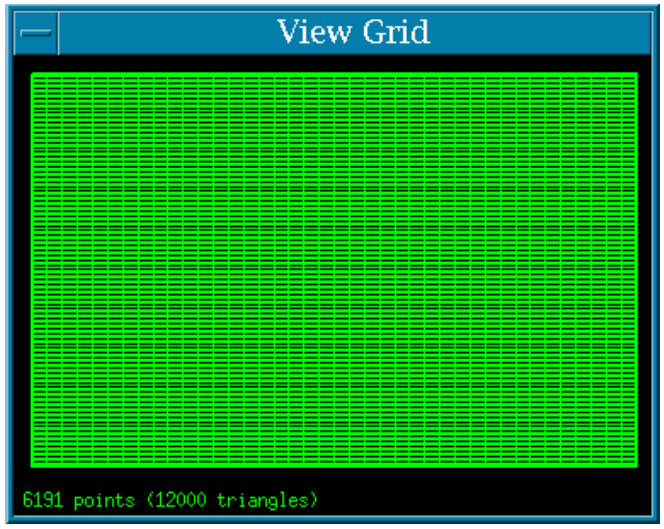
To generate Extract statement

What is a simulation grid

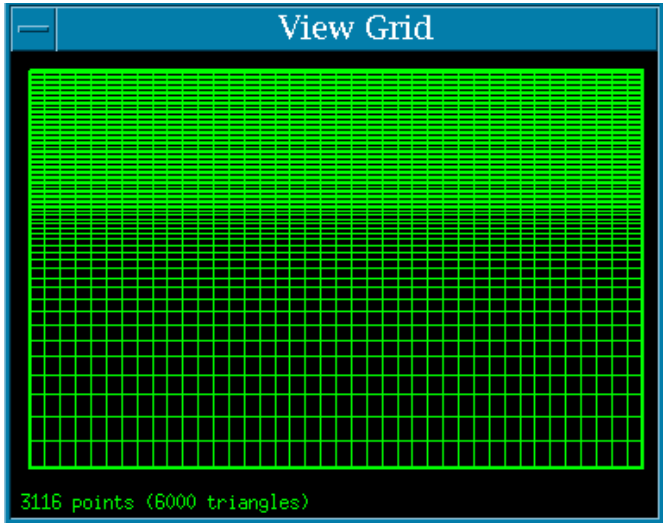
The simulation grid represents the points (***nodes***) of the structure where the model equations are solved. Therefore the correct specification of a grid is critical in process simulation.

The number of nodes in the grid has a direct influence on simulation accuracy and time.

A finer grid should exist only in the critical areas of the simulation structure (where ion implantation will occur or where *p*-*n* junction will be formed).



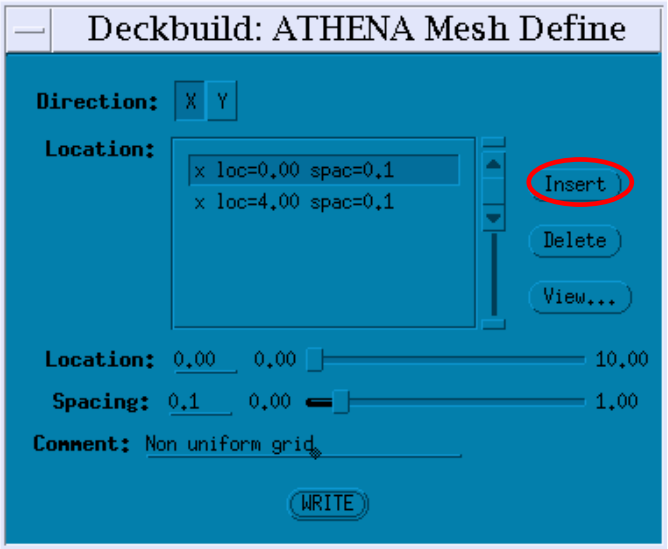
Uniform grid
fine into unnecessary regions



Non uniform grid
fine only into critical regions

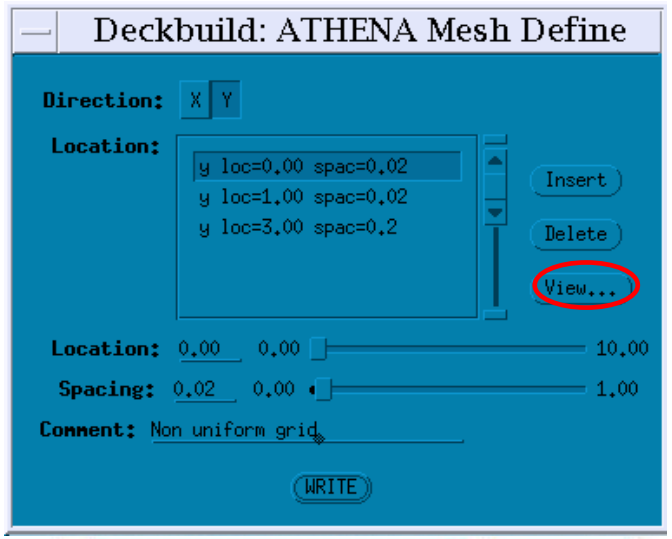
Defining simulation grid (1)

Open the ***Commands*** menu and select ***Mesh Define...***



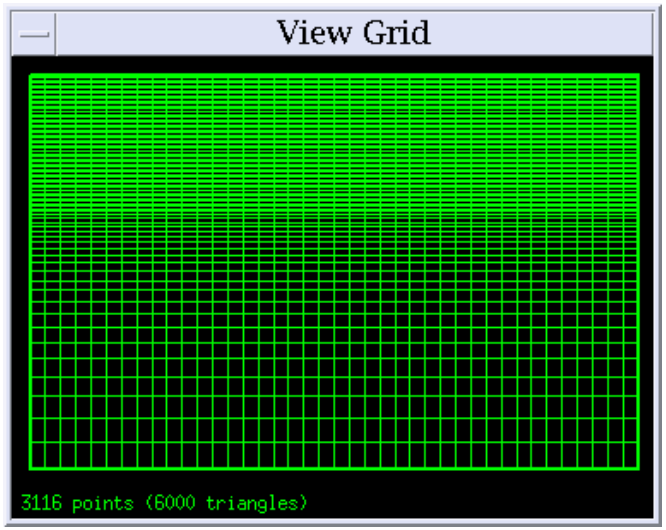
- Units are Microns
- In the Mesh Define Menu click on the Location field and enter a value of 0.0.
- Then, click on the Spacing field and enter a value of 0.1.
- Finally, click on the *Insert* button and the line parameters will appear in the scrolling list.
- Set the location of a second X line to 4.0 with the same spacing of 0.1.

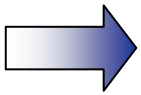
- In the same way, set the values for the Y direction as showed in the figure.
- Before writing the mesh information into the input file, select the *View...* button.

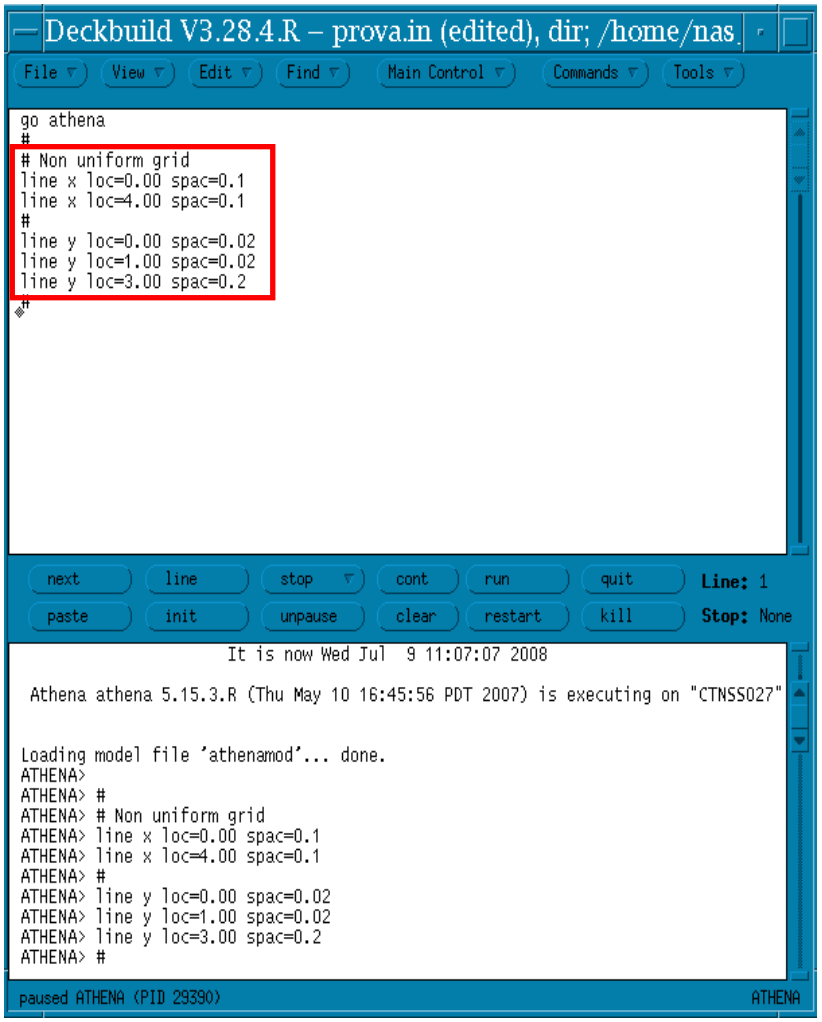


Defining simulation grid (2)

Pressing the *View…* button a preview of the rectangular grid will appear.







- Write the Mesh Define information to the input file by pressing the *Write* button.
- A set of command lines will appear in the Deckbuild Text Subwindow. The first line (*go Athena*) tells Deckbuild that the following file should be run by Athena.

Question 2

The simulation grid:

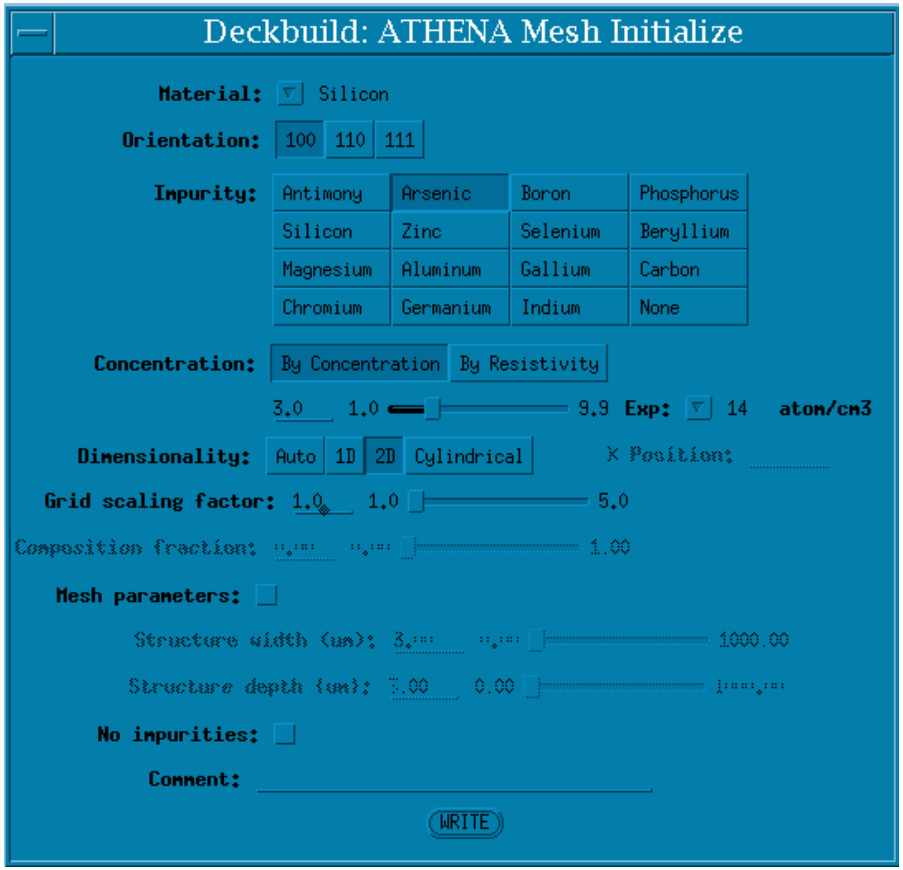
a) should be uniform in all device regions

b) has direct influence on simulation time

c) must not be necessarily defined in the input file

Defining initial substrate (1)

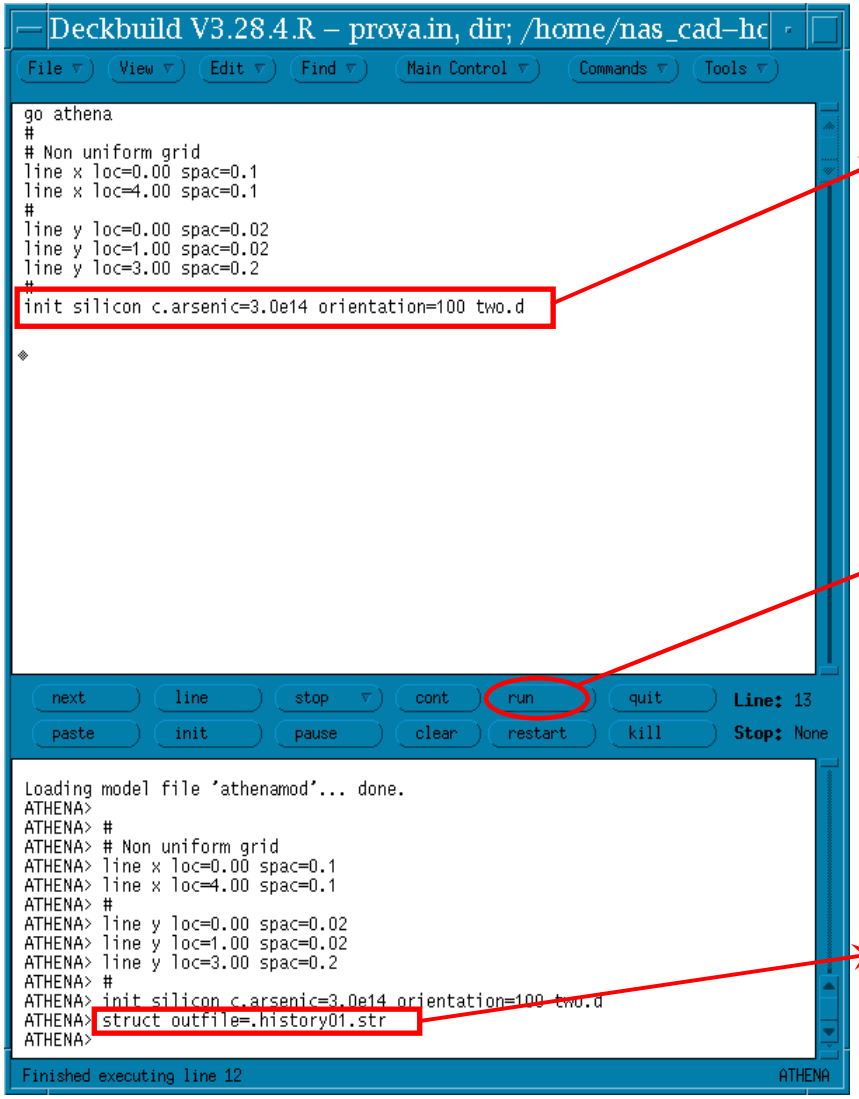
Choose the ***Mesh Initialize*** item in the ***Commands*** menu



- In the Mesh Initialize popup set the material, the orientation and the background doping.
- Substrate concentration can be specified by Resistivity (in Ohm*cm) or by Concentration in atom/cm^3.
- In the Dimensionality field click on the 2D button to run the simulation in a two-dimensional calculation (*).
- The mesh initialization information can be written into the file by pressing the *Write* button.

* 2D mode is used in this tutorial to give an idea of 2D grid generation and manipulation. In most cases, however, the Auto default shouldn't be changed. Athena will begin in 1D and will automatically switch to 2D mode at the first statement that disrupts the lateral uniformity of the device structure. This generally results in a considerable saving of computation time.

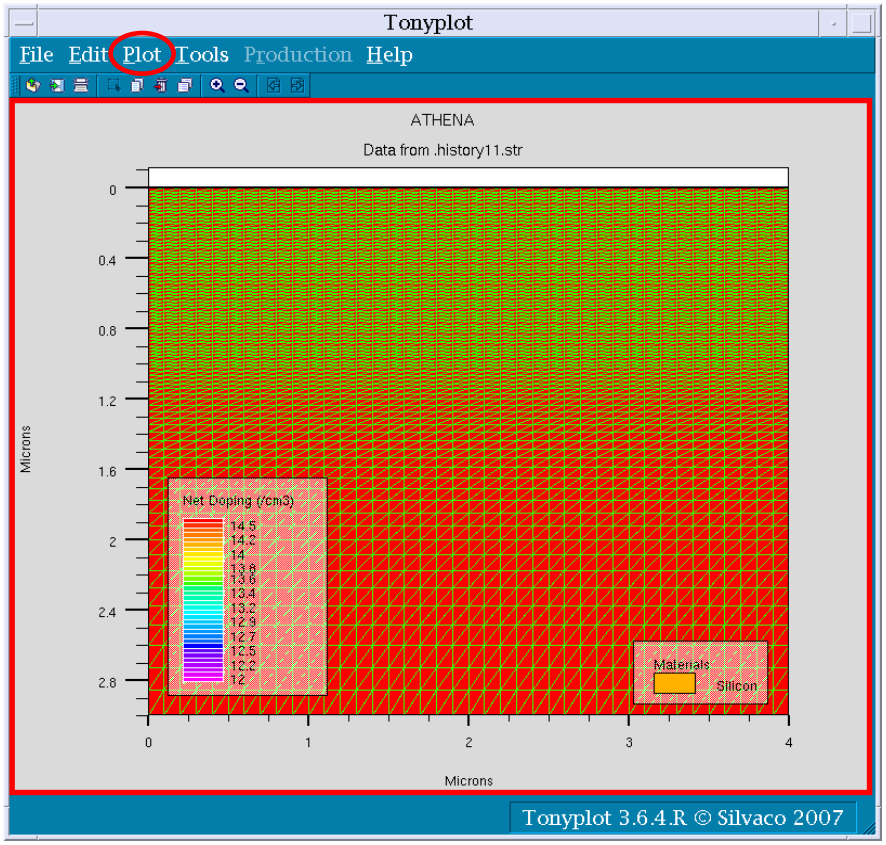
Defining initial substrate (2)



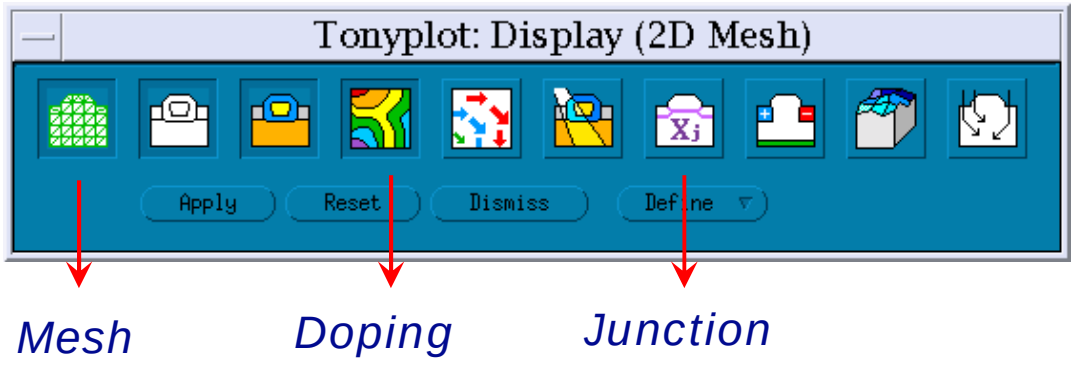
- Pressing the *Write* button the corresponding command line will appear in the Deckbuild Text Subwindow.
- Press the *Run* button to run Athena and to obtain the initial structure.
- Through the history function a structure file is automatically saved. The STRUCT OUTFILE line is generated in the Deckbuild Output Subwindow.

Visualizing initial structure

- Highlight with the mouse the name of the structure file (*.history01.str*)
- Click on the ***Tools*** button.
- Select ***Plot → Plot structure***



- Deckbuild will run ***Tonyplot***
- In Tonyplot window click on the ***Plot*** menu button and select ***Display***.
- In the Display popup select the *Mesh* and *Doping* buttons to display the initial triangular grid and the substrate doping.

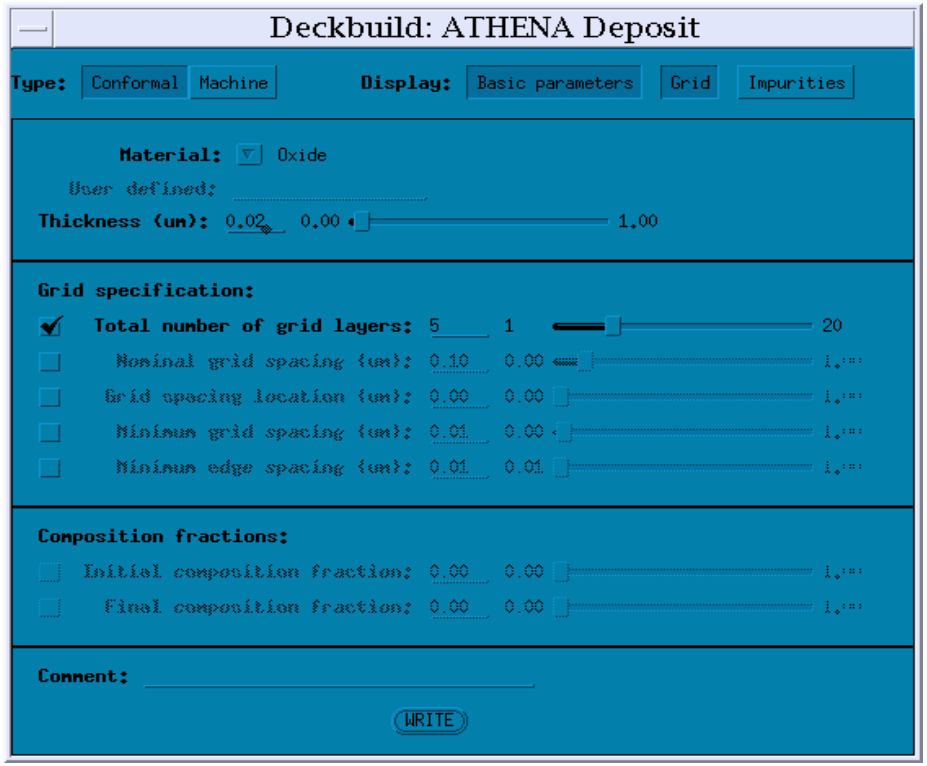


Layer deposition (1)

The previous INIT statement created the <100> silicon region of 4.0µm x 3.0µm size, which is uniformly doped with arsenic concentration of 3e14 atom/cm^3.

This simulation structure is ready for any process step (deposition, implantation, diffusion, …).

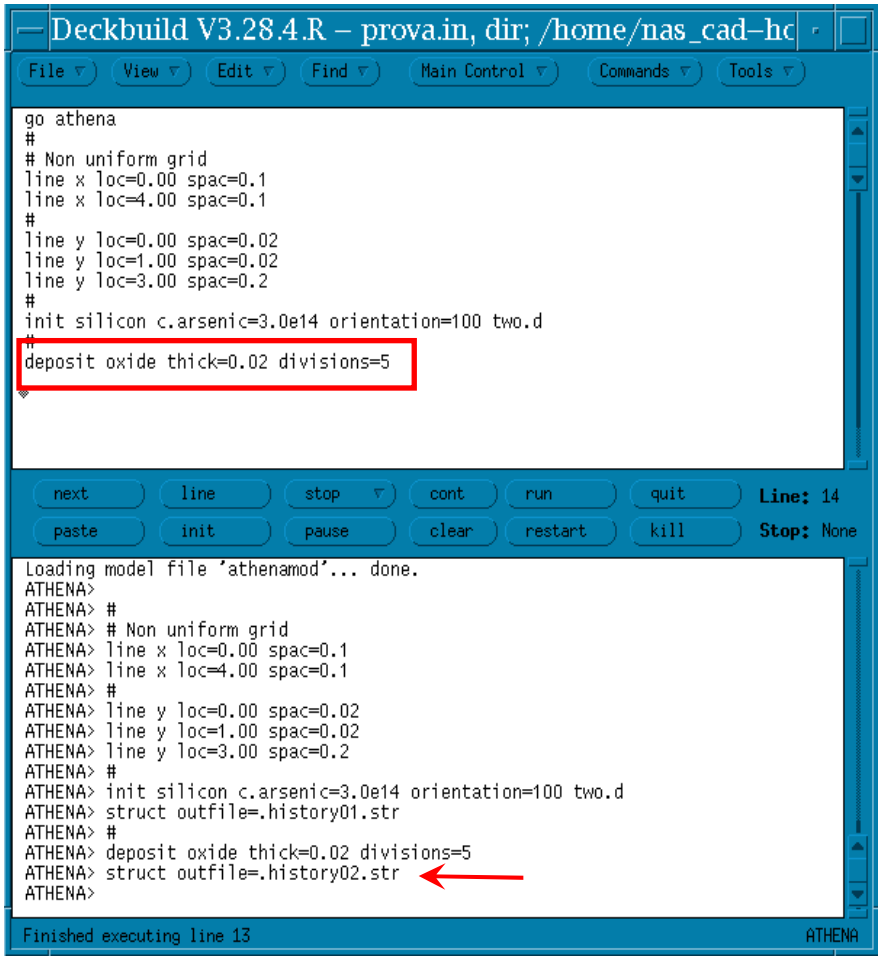
Select the items ***Process*** → ***Deposit*** → ***Deposit...*** from the ***Commands*** menu

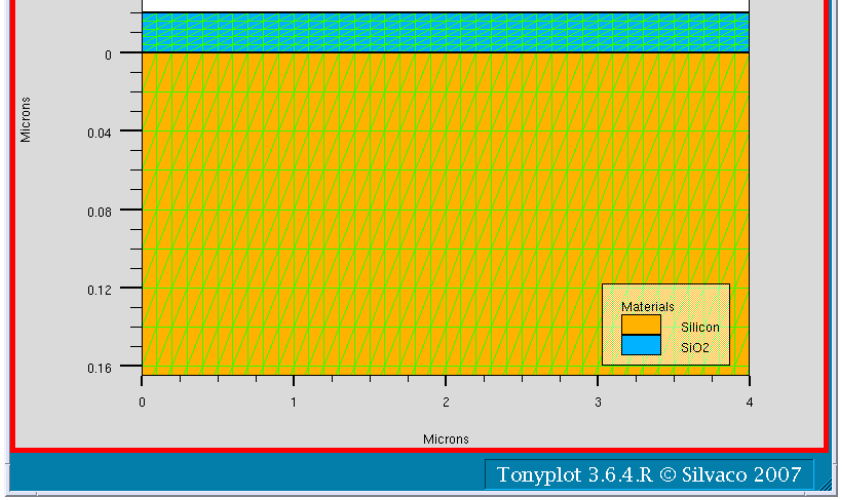


- Select Oxide from the *Material* menu and set its thickness to 0.02 µm.
- Set to 5 the *Total number of grid layers* (it is always useful to set several grid layers in a deposited layer).
- Click on the *Write* button.

Layer deposition (2)

Pressing the *Write* button, the corresponding command line is showed in the Deckbuild Text Subwindow. The history file can be displayed by Tonyplot to check the structure step by step.

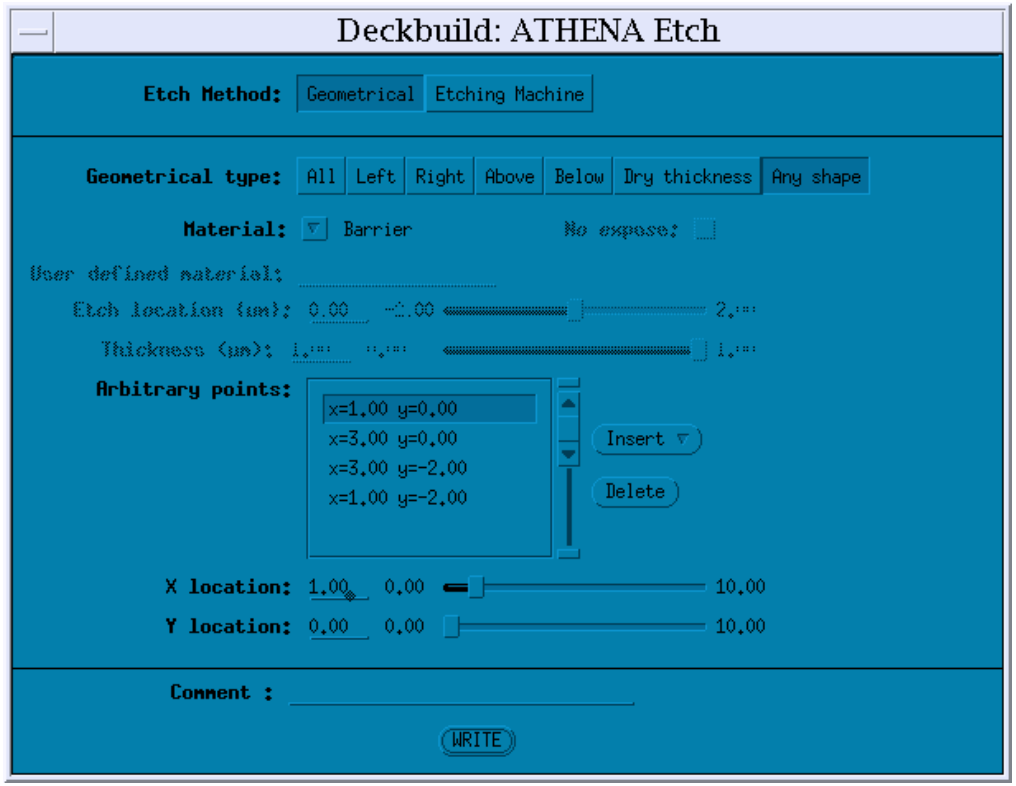




Geometrical etching (1)

The next step in this process simulation is to define an implant window. To do this, first deposit a layer of barrier (or photoresist). Then perform the geometrical etching of the layer where we want to implant. To set a geometrical etch step:

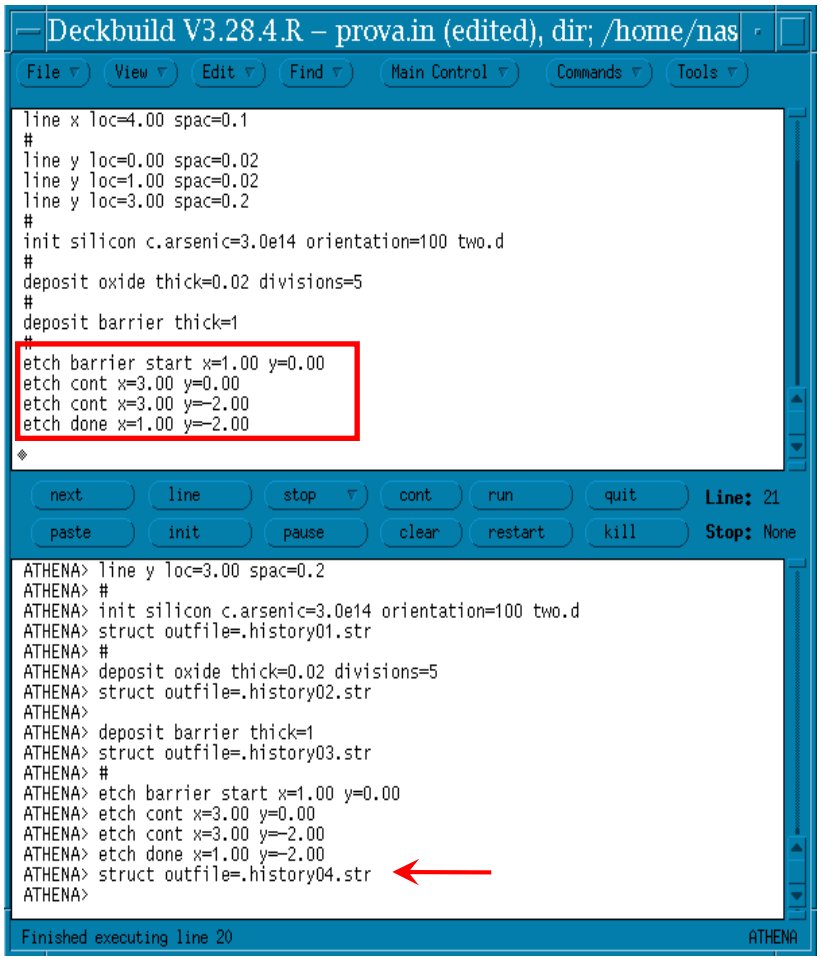
Select ***Process*** → ***Etch*** → ***Etch...*** from the ***Commands*** menu.

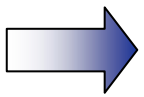


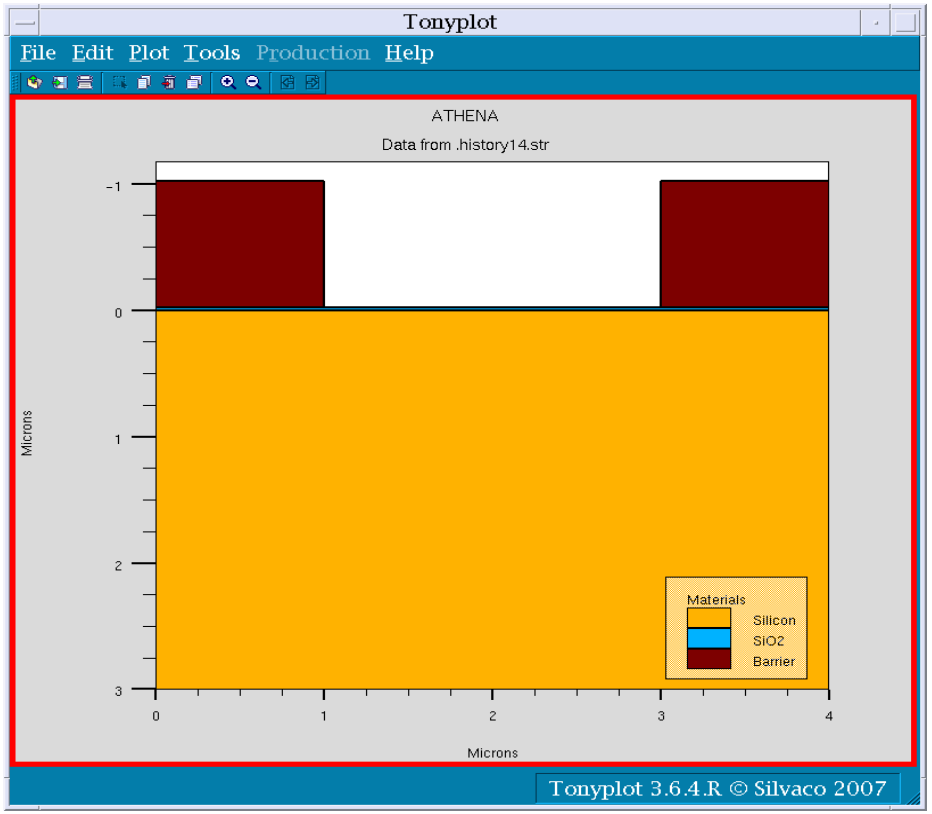
- Select barrier from the *Material* menu.
- An arbitrary shape of the etching can be obtained by using the *Any Shape* button.
- Specify X and Y locations of the four vertices of the rectangle you want to eliminate.
- Click on the *Write* button.

Geometrical etching (2)

Pressing the *Write* button, four etch lines will be inserted into the input file. The structure created by this etch statement is shown in the plot on the right.



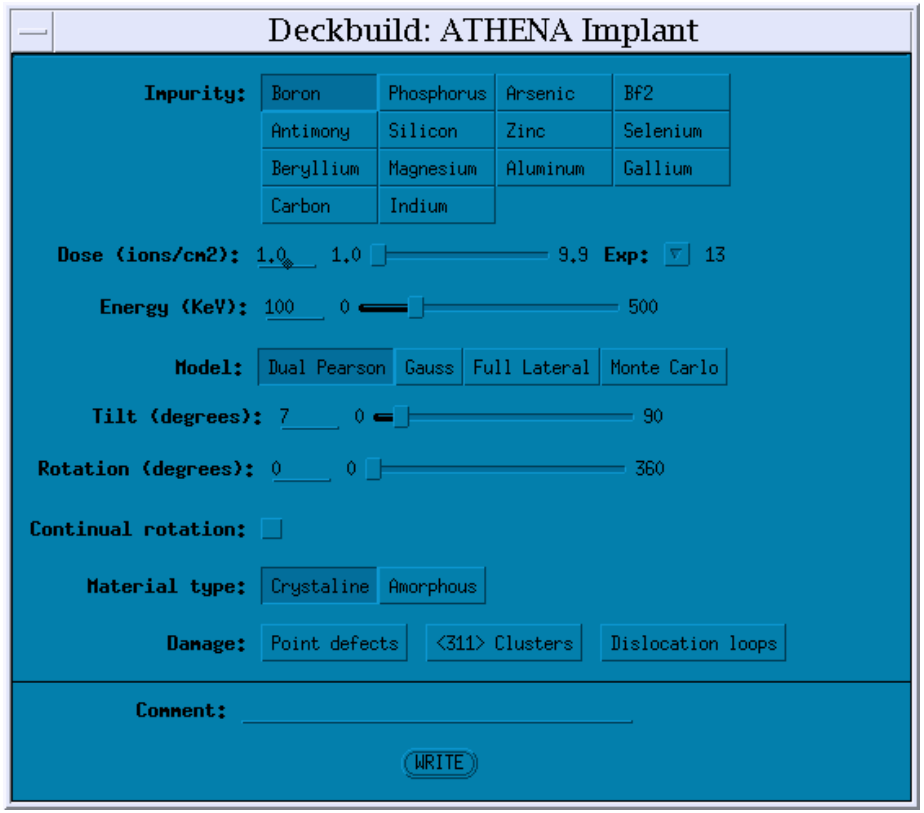




Ion implantation (1)

The implant statement can be set by using the Implant Menu. To open this menu:

Select ***Process*** → ***Implant...*** in the ***Commands*** menu



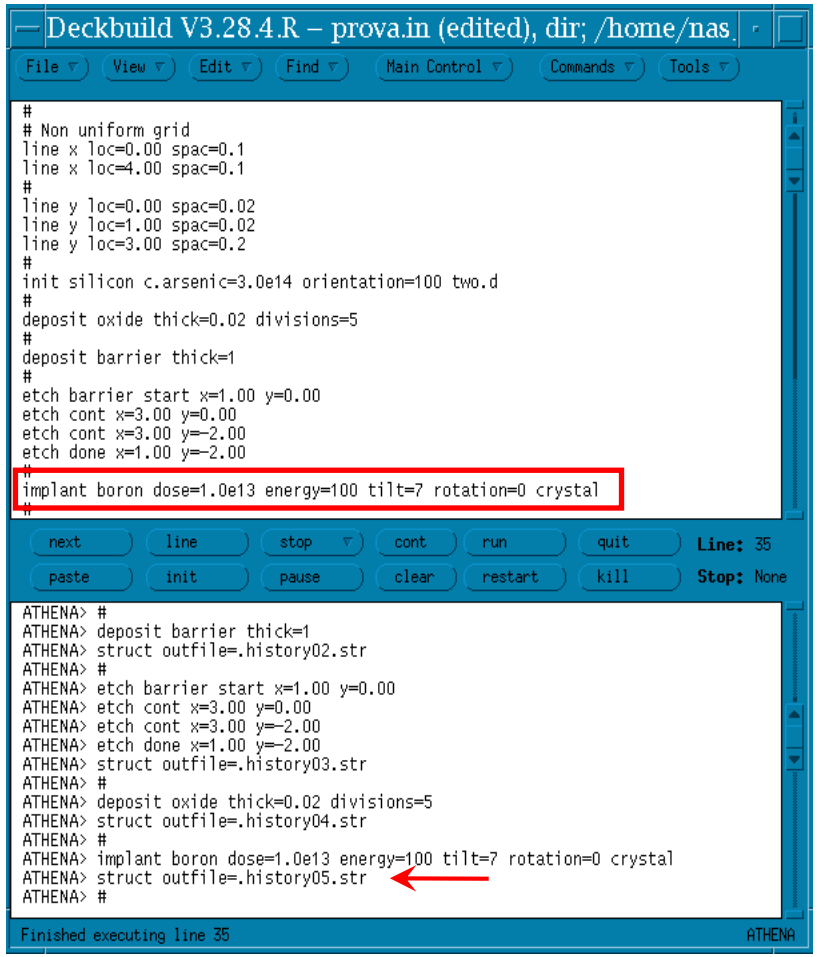
The fundamental parameters that can be specified are:

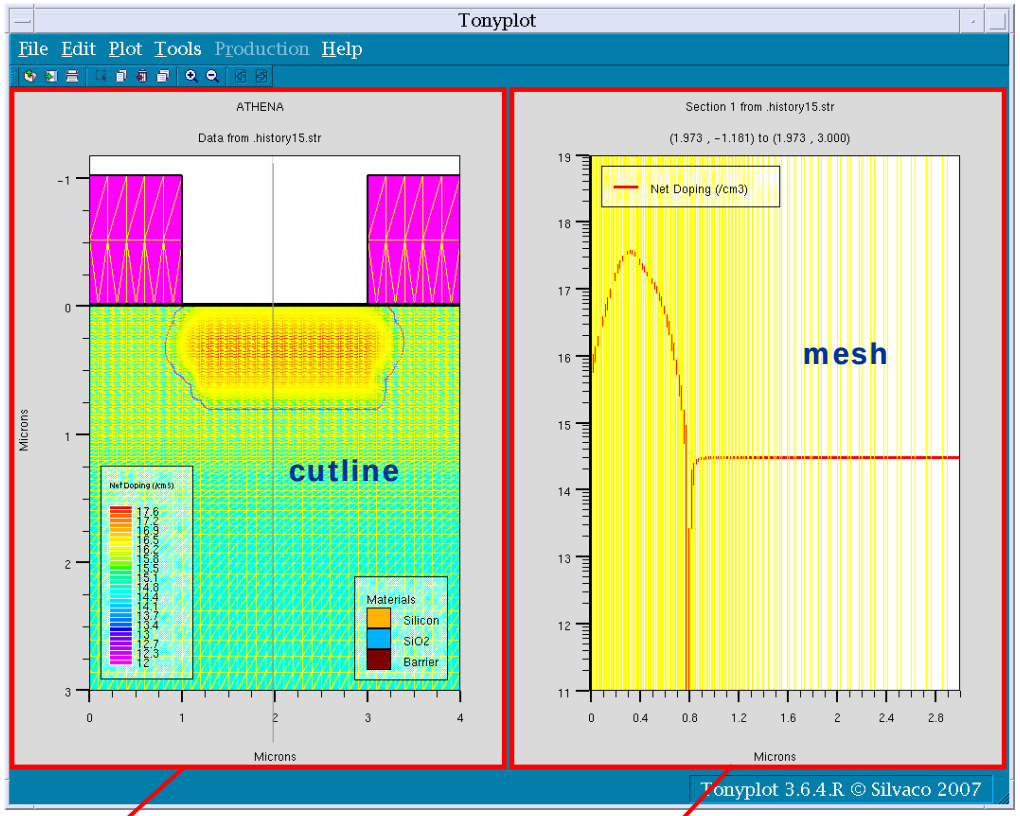
- Name of implant impurity
- Implant dose (in atm/cm^2)
- Implant energy (in KeV)
- Tilt and rotation angles (in degrees)
- Material type (crystalline or amorphous)

The available implant models will be discussed in the next section. By default the analytic model is selected.

Ion implantation (2)

Pressing the Write button the implant statement appears in the input file





2D profile after the implant step

1D profile obtained performing a vertical cutline on the 2D structure

Question 3

The implantation step:

a) must always be performed in 2D mode

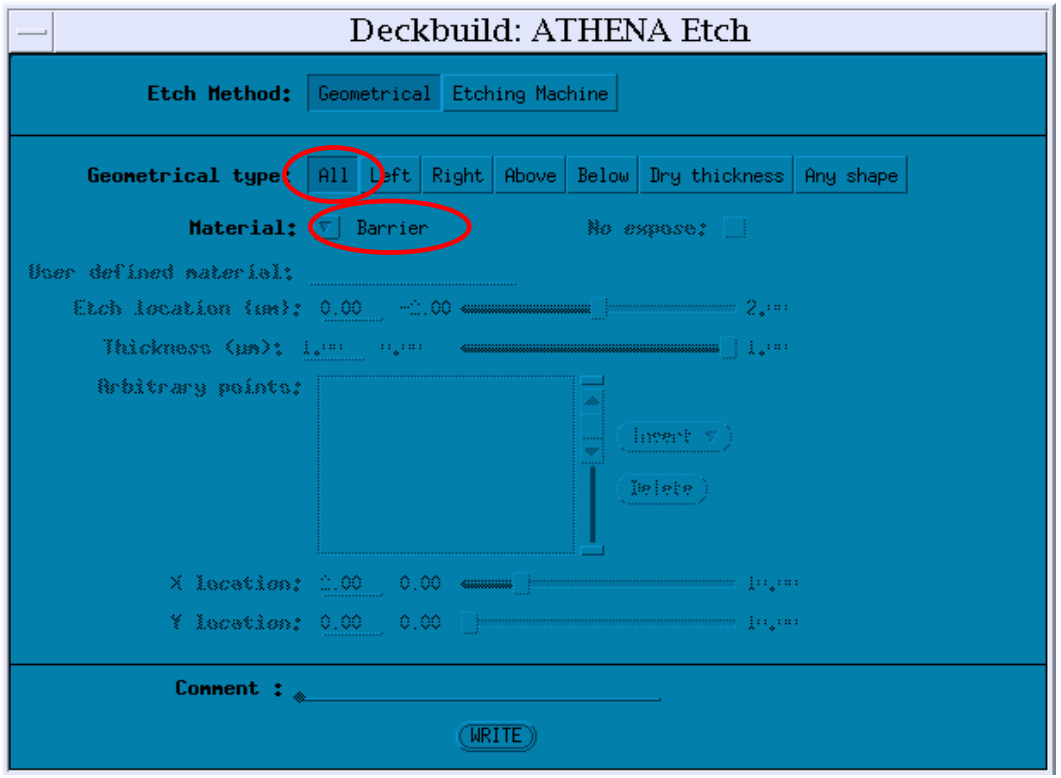
b) can be performed only on crystalline silicon

c) requires the specification of implant dose and energy

Removing implant mask

Before the diffusion step it is necessary to remove the barrier mask performing an etching process.

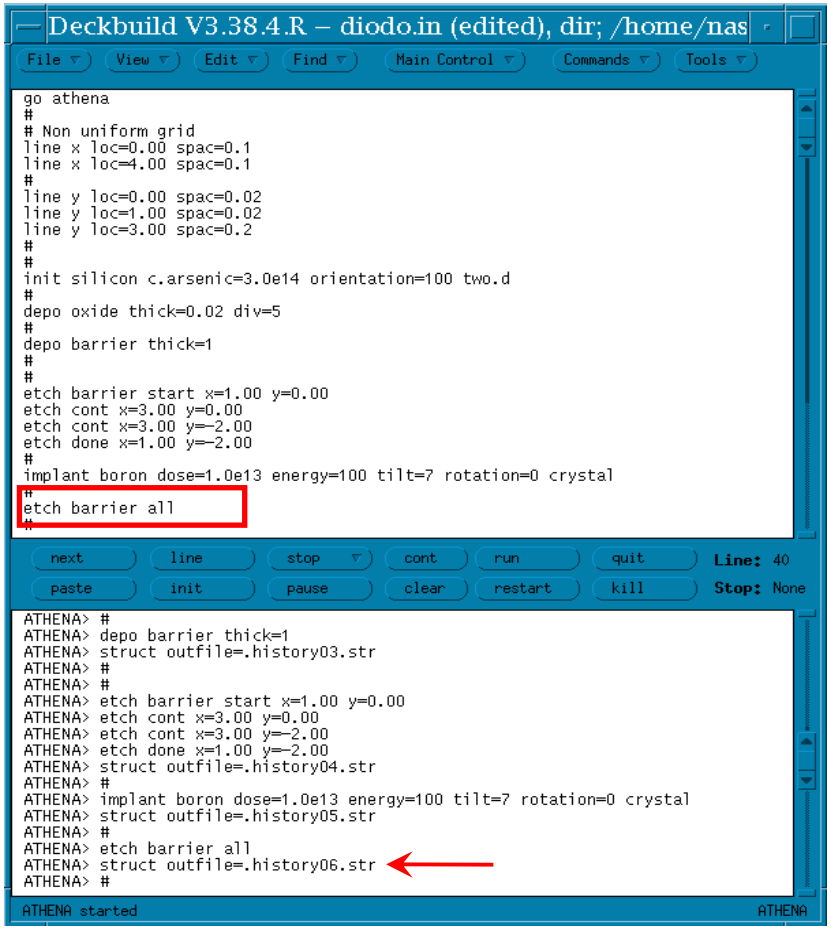
To do this select ***Process*** → ***Etch*** → ***Etch...*** from the Commands menu.

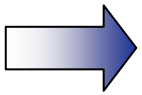


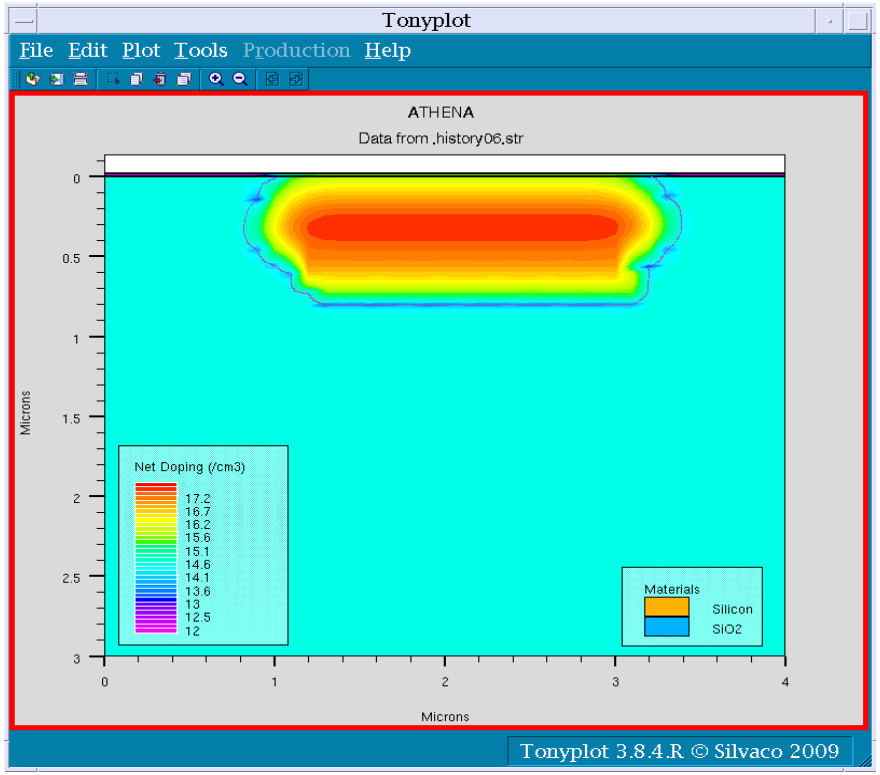
- Select *Barrier* from the Material menu.
- Select *All* from the Geometrical type menu
- Click on the *Write* button.

Removing implant mask (2)

In this way the statement that removes all the barrier material from the structure appears in the input file.



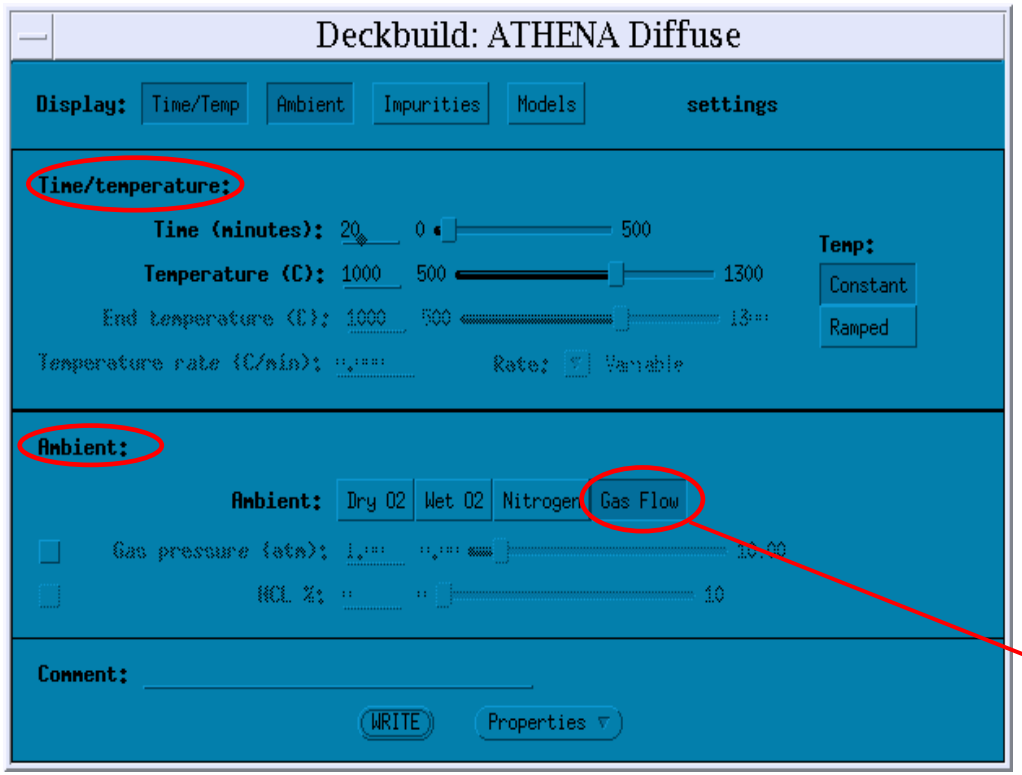




Diffusion (1)

Select ***Process*** → ***Diffuse...*** in the ***Commands*** menu

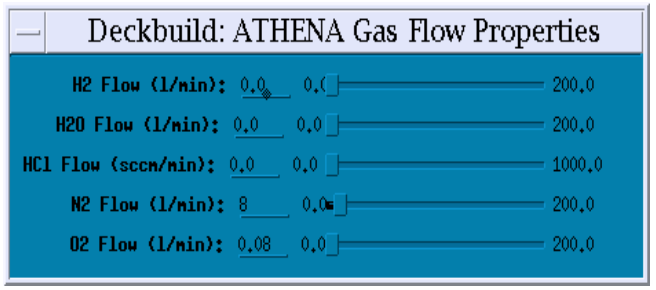
The Diffuse menu has four sections. Only the Time/Temperature and Ambient fields appear initially. The Impurities and Models fields appear only when the corresponding check boxes are selected.



The minimum set of diffusion parameters is:

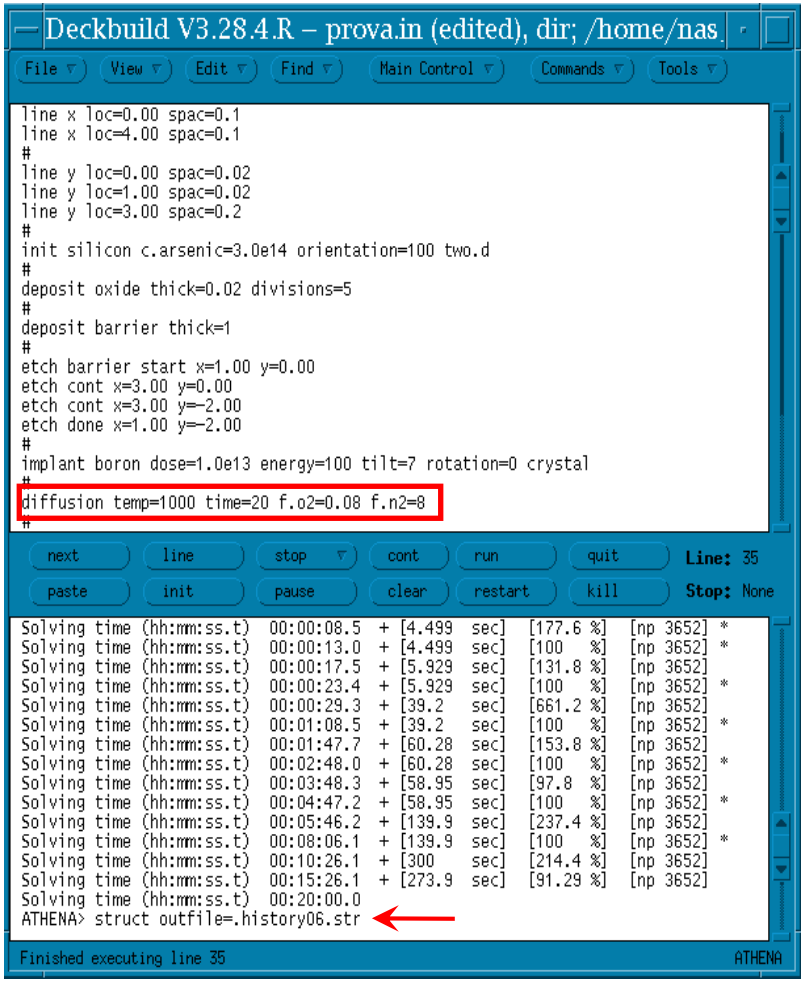
- Time (minute is the default)
- Temperature (in Celsius degree)
- Gas pressure (default=1 atmosphere)

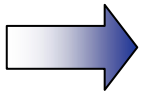
If the ambient is a mixture of oxidants, select the *Gas Flow* button in the ambient section and an additional Menu will appear.

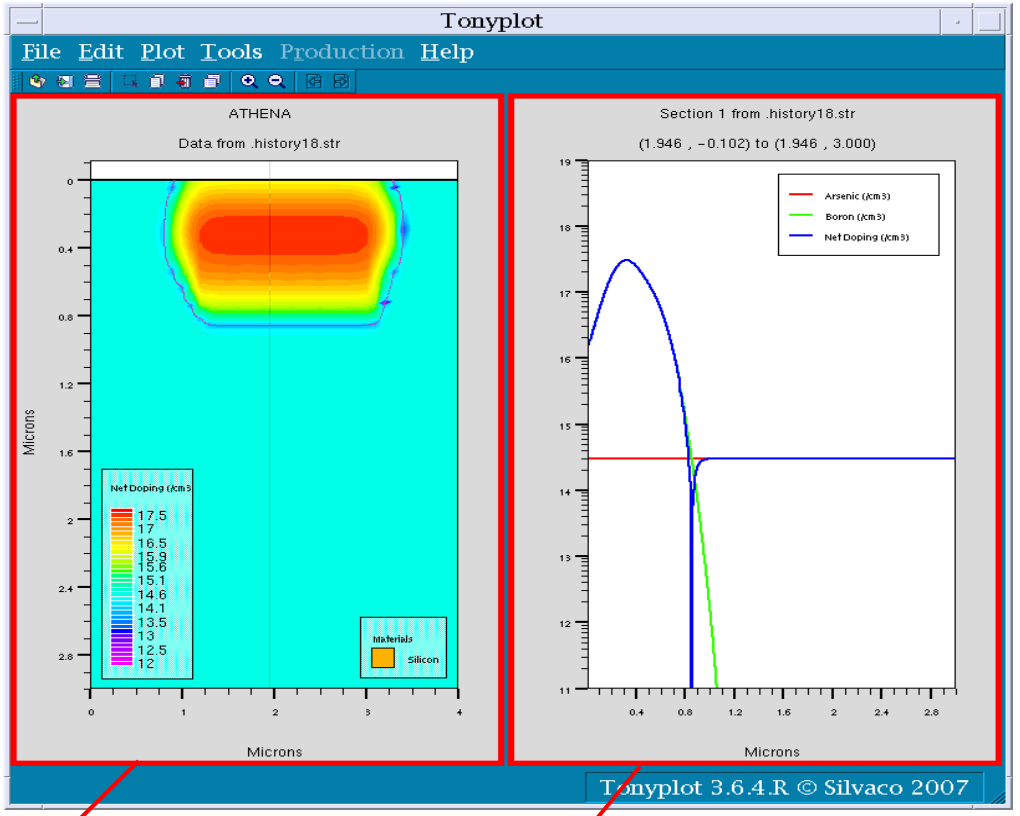


Diffusion (2)

Pressing the write button the corresponding command line will appear in the Deckbuild text window.







2D profile after the diffusion step

1D profile obtained performing a vertical cutline on the 2D structure

Question 4

The diffusion step:

a) doesn't allow to specify a mixture of oxidants

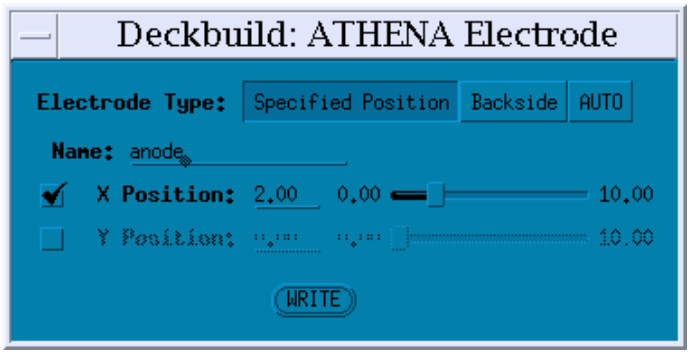
b) can be performed only after an implant step

c) requires time and temperature to be specified

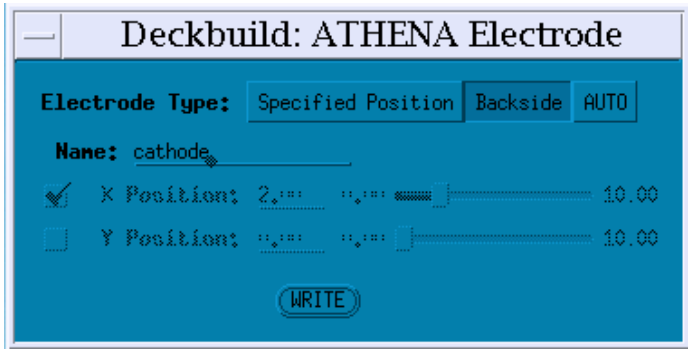
Specification of Electrodes (1)

The ultimate goal of an Athena simulation is to create a device structure that can be used by the device simulator for electrical characterization. The locations of electrodes can be specified both in Athena and Atlas. Athena can attribute an electrode to any *metal*, *silicide*, or *polysilicon* region. After creating the aluminum contact, by using deposition and etching, open the Electrode Menu:

Select ***Structure*** → ***Electrode...*** in the ***Commands*** menu



- To set the anode electrode select the *Specified Position* button, write the X position and the name.



- To specify the backside electrode, select *Backside* and type the name cathode.

Specification of Electrodes (2)

Pressing the *Write* button, two command lines will be inserted into the input file.

Deckbuild V3.28.4.R – prova.in (edited), dir; /home/nas

File View Edit Find Main Control Commands Tools

```
#
deposit oxide thick=0.02 divisions=5
#
deposit barrier thick=1
#
etch barrier start x=1.00 y=0.00
etch cont x=3.00 y=0.00
etch cont x=3.00 y=-2.00
etch done x=1.00 y=-2.00
#
implant boron dose=1.0e13 energy=100 tilt=7 rotation=0 crystal
#
diffusion temp=1000 time=20 f.o2=0.08 f.n2=8
#
deposit aluminum thick=0.1
#
etch aluminum left p1.x=1.50
etch aluminum right p1.x=2.50
#
electrode name=anode x=2.00
electrode name=cathode backside
#
```

next line stop cont run quit **Line:** 35

paste init pause clear restart kill **Stop:** None

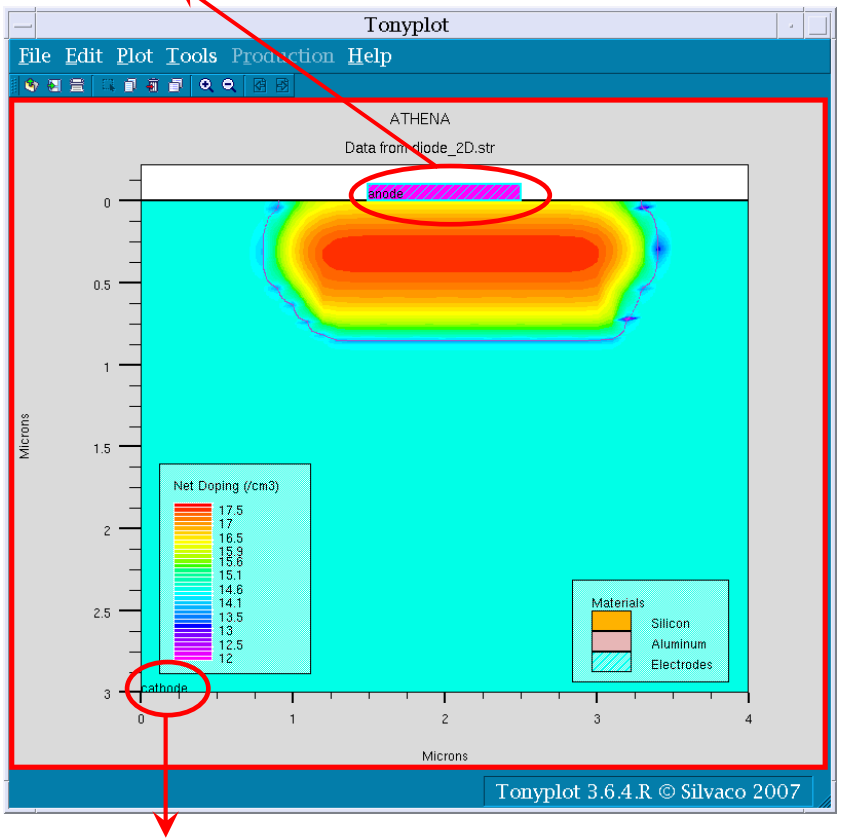
```
ATHENA> #
ATHENA> etch aluminum left p1.x=1.50
ATHENA> struct outfile=.history08.str
ATHENA> etch aluminum right p1.x=2.50
ATHENA> struct outfile=.history09.str
ATHENA> #
ATHENA> electrode name=anode x=2.00

Note:   Material at chosen location is aluminum. Electrode is set
        for this region. Location is x = 2.000000


ATHENA> struct outfile=.history10.str
ATHENA> electrode name=cathode backside
ATHENA> struct outfile=.history11.str
ATHENA> #
```

Finished executing line 35 ATHENA

anode



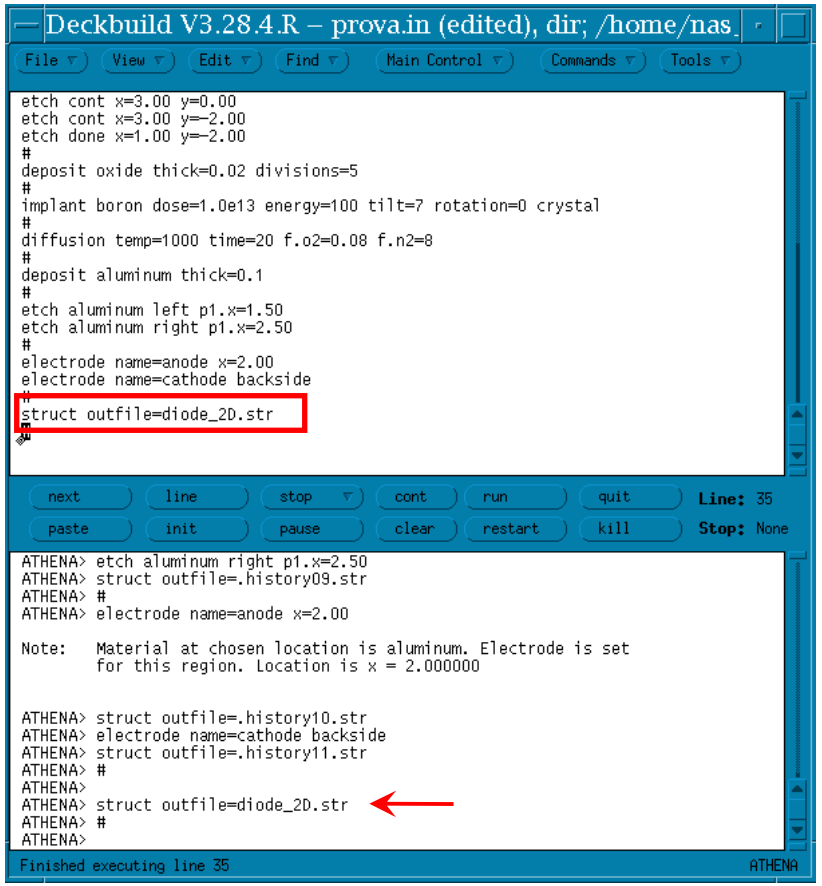
cathode

Saving a structure file

If you want to save the structure information generated after some key process steps

Select ***Commands → File I/O....***

- Specify a file name (the file extension *.str* is recommended) and click on the *Save* button.
- Press the *Write* button and the corresponding line will appear in the input file.

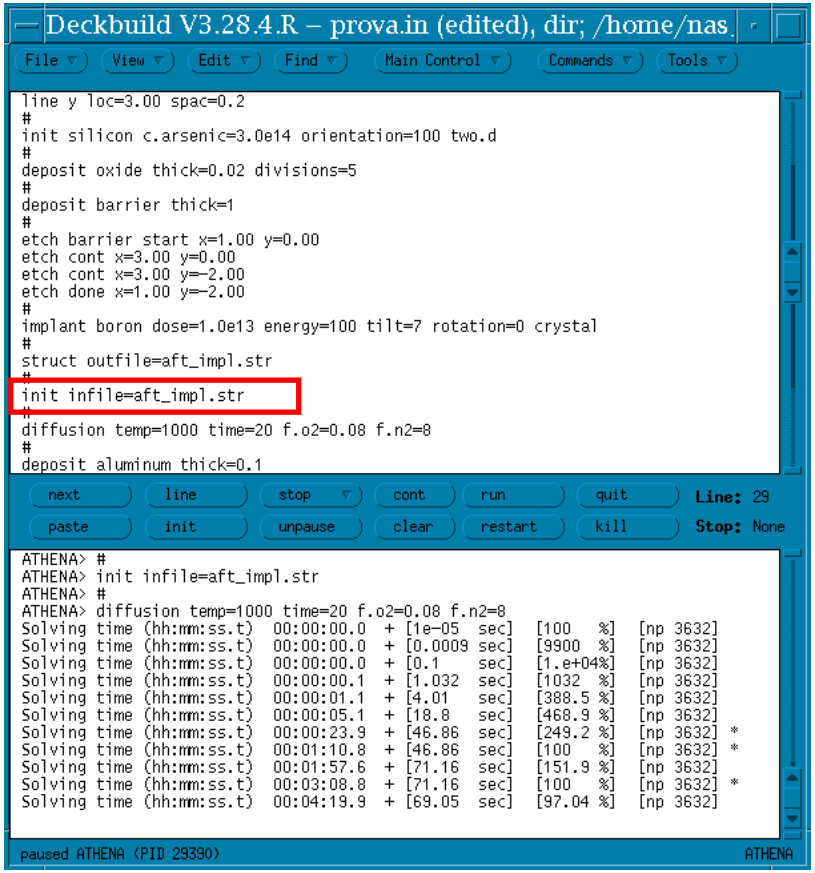


Restarting Athena simulation

A structure file can be used to initialize an Athena input file for further processing. To reload a structure file

Select ***Commands → File I/O....***

- Press the *Load* button and insert the file name.
- Press the *Write* button and the corresponding line will appear in the input file (*).



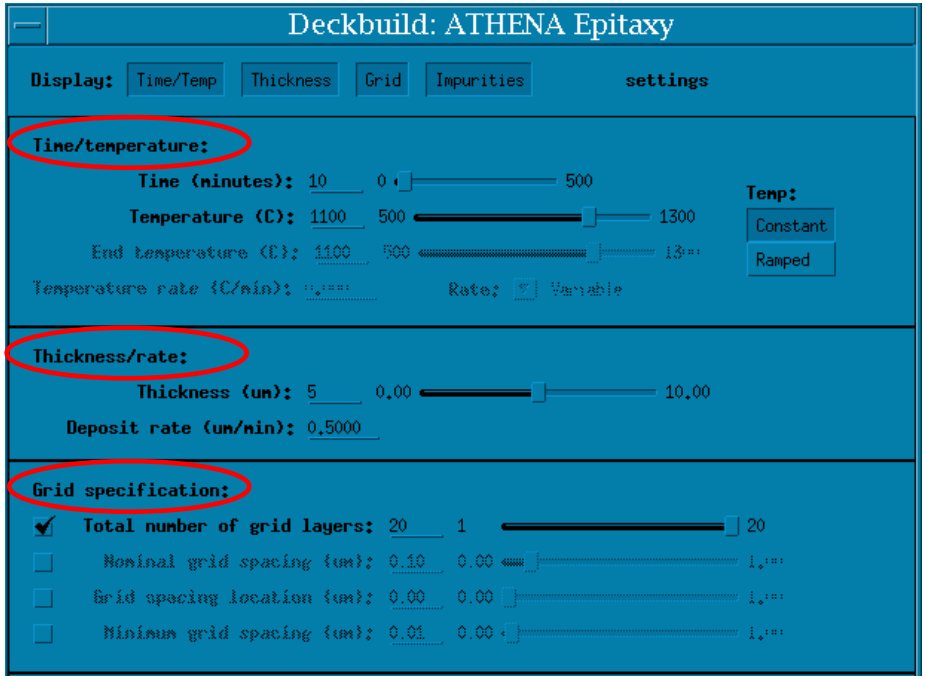
* Note that only the structure will be reloaded. Any parameters or coefficients that were set during previous simulations must be reset if they are needed.

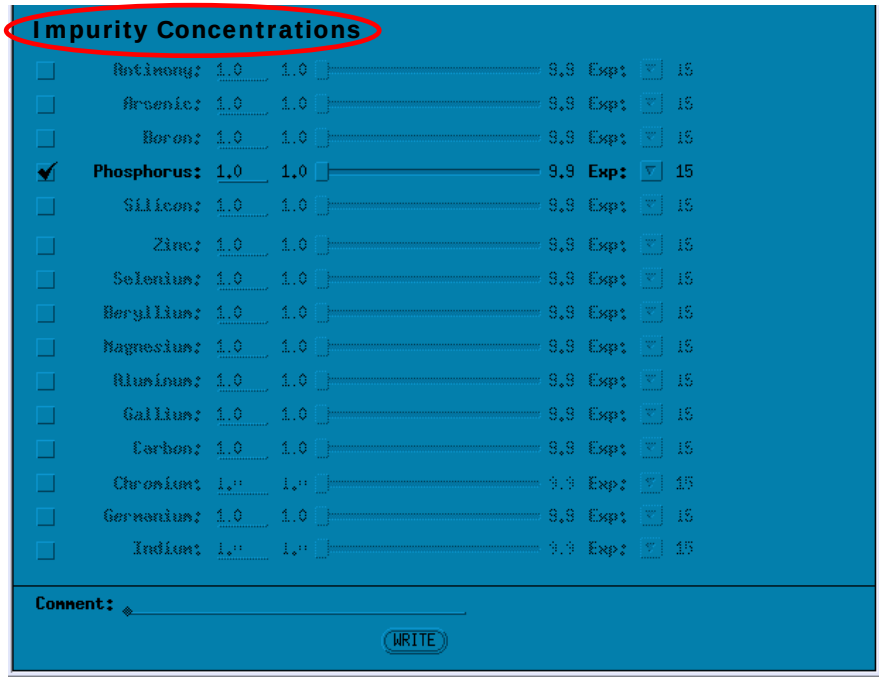
Epitaxy Process

Epitaxy is modeled as a combination of **deposit** and **diffuse** processes. Autodoping from a highly doped buried layer into a lightly doped epitaxial layer can be simulated.

Select ***Process*** → ***Epitaxy*** in the ***Commands*** menu.

The Epitaxy Menu consists of four sections:





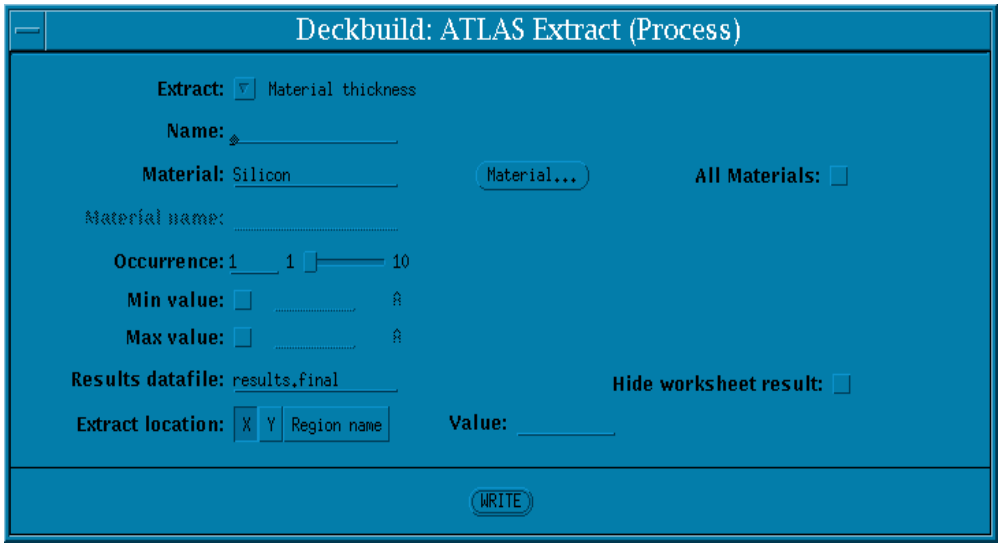
The command line of a typical epitaxial step is:

EPITAXY TIME=10 TEMP=1100 THICKNESS=5 DIVISIONS=20 C.PHOSPHOR=1.0E15

Extract function (1)

Deckbuild has a built-in language that allows extraction of physical and electrical quantities from simulation results. The result of all extract expressions is either a single value or a two-dimensional curve. To place an extract statement:

Select ***Extract…*** in the ***Commands*** menu

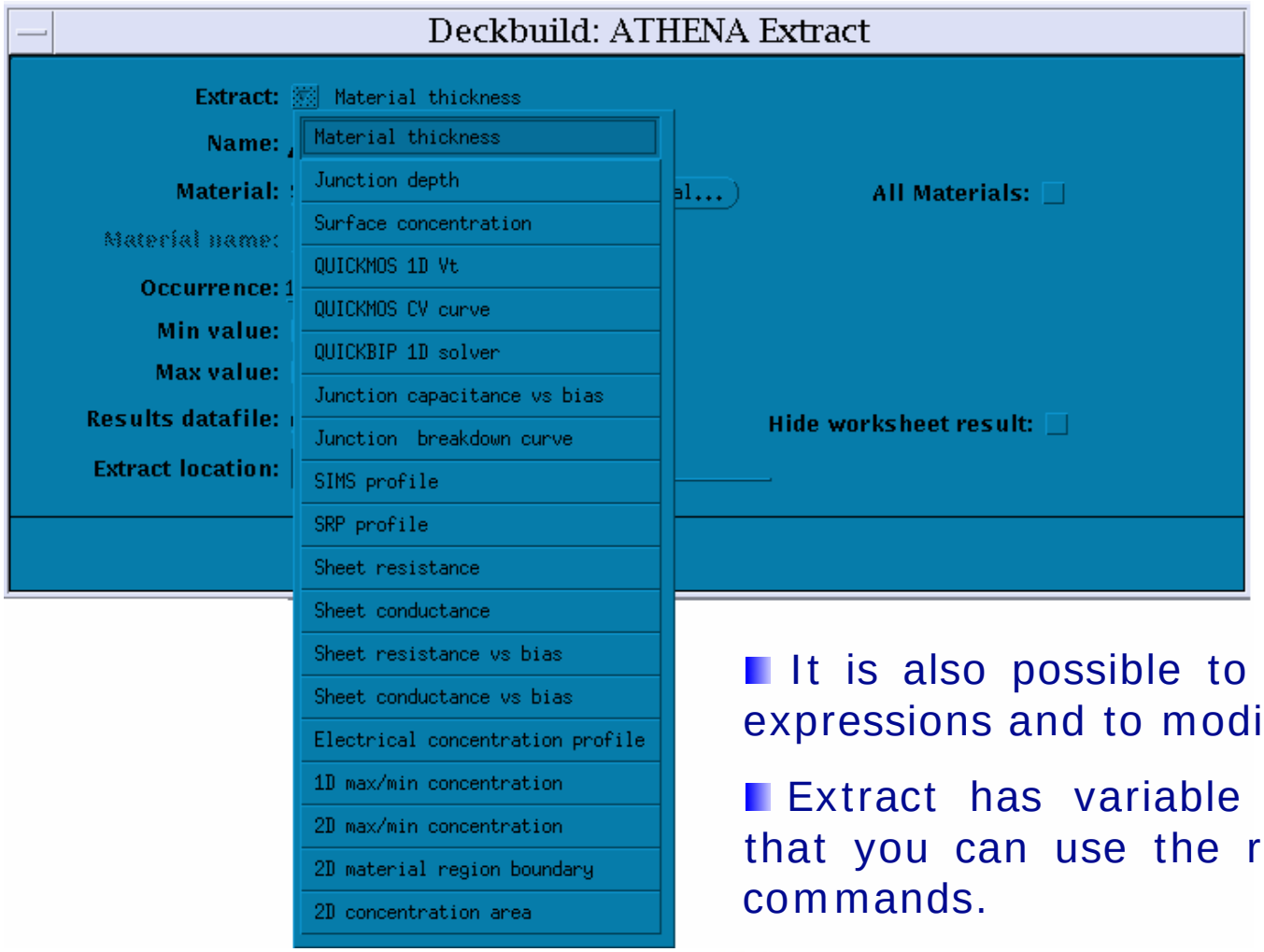


- In the Extraction popup, choose the desired extract routine from the Extract field.
- The popup will display different items depending on the chosen routine.
- Enter the required information for each item on the popup.

An extract name is always required. By default, all extract results are written to a file named *results.final*. But the Results datafile field allows you to specify the results file for each individual extract statement.

Extract function (2)

It is possible to create customized expressions or choose from a number of ***standard routines*** provided for the process simulators.



- It is also possible to take one of the standard expressions and to modify it to suit needs.
- Extract has variable substitution capability so that you can use the results of previous extract commands.

Question 5

In a process simulation:

a) only one structure can be saved at the end of the simulation input file

b) intermediate structures can be saved and displayed by Tonyplot

c) intermediate structures can be saved, but not displayed

Choosing models in Athena

In dopant involving simulation the use of the **appropriate model** is critical for simulation accuracy.

A correct choice of models is needed for **implantation**, **diffusion** (or rapid thermal annealing) and **oxidation**.

The key to accurately simulate any dopant related process is to correctly account for **damage** in the semiconductor.

The simulation time is greater if the models are more complicated.

A **compromise** between simulation accuracy and simulation time can always be achieved.

Implant models

Athena uses analytical and statistical techniques to model ion implantation

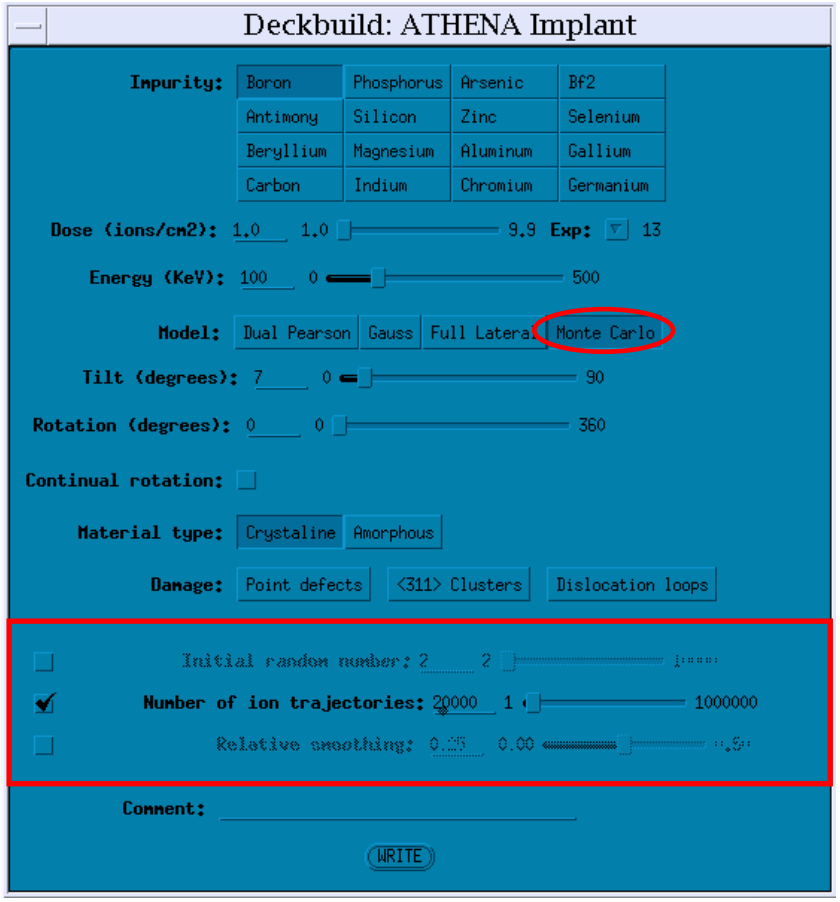
- ***Analytical models*** are based on the reconstruction of implant profiles from the calculated or measured *distribution moments*.

- ***Statistical models*** use the physically based *Monte Carlo calculation* of ion trajectories to calculate the final distribution of stopped particles.

Model	Syntax	Assumption	Recommendation
Gauss	*gauss*	Analytical	- Generally it is **inadequate** because real profile are asymmetrical in most cases.
Pearson IV **Dual Pearson IV (default)**	*pearson*	Analytical	- For profiles heavily affected by **channel**. - Sims-Verified Dual Pearson (SVDP) implant models for B, BF2, P, As.
Monte Carlo **BCA**	*montecarlo* *bca*	Statistical	- When channeling is not described by SVDP. - **High or very low energy**.

Monte Carlo model

A beam of fast ions entering crystalline or amorphous solid is slowed down and scattered due to nuclear collisions and electronic interaction. The paths of the individual moving particles and their collisions are modeled by means of the **Binary Collision approximation** (BCA).



User need to specify some optional parameters to control Monte Carlo calculation. The fundamental one is the **Number of ion trajectories**.

- The default is 1,000 for 1D structures and 10,000 for 2D structures.
- The accuracy increases with the number of ions, but also the execution time increases. Therefore a compromise must be achieved.

Two dimensional implant profile

Athena calculates ***2D implant profiles*** by using the following approximation:

$$f_{2D}(x,y) = f_l(y) \cdot f_t(x)$$

Longitudinal function $f_l(y)$: Gaussian (default), Pearson, Dual-Pearson

Depth-independent *transversal function* $f_t(x)$

Lateral standard deviation

$$LAT.RATIO1 = \frac{lateral\ std\ dev}{proj\ range} = 1\ (default)$$

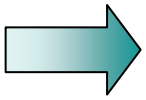
$$LAT.RATIO2\ (2^{nd}\ \text{Pearson}) = 0.2\ (default)$$

The **`print.mom`** parameter in the `IMPLANT` statement prints the calculated (or extracted from the tables) moments into output.

Diffusion models (1)

All diffusion models follow the same generic mathematical form of a ***continuity equation***.

A continuity equation merely expresses particle conservation.



The rate of change with time of the number of particles in a unit volume must equal the number of particles that leave that volume through diffusion, plus the number of particles that are either created or annihilated in the volume due to various source and sink terms.

This basic continuity equation for the diffusion of some particle species (C) in a piece of semiconductor material is a simple Second Order Fick's Equation:

$$\frac{\partial C_{ch}}{\partial t} = -\nabla J_A + S$$

where:

- C_{ch} is the total particle (chemical) concentration
- J_A is the flux of mobile particles
- S accounts for all source and sink terms.

Diffusion models (2)

In semiconductor diffusion problems, there are generally two contributors to the particle flux:

- An ***Entropy Driven*** term that is proportional to the concentration gradient of mobile particles. The coefficient of proportionality, DA, is called the diffusivity.
- A ***Drift*** term that is proportional to the local electric field.

The Flux Term J_A can be written as:

$$J_A = -D_A \nabla C_A + C_A \mu E$$

where:

- C_A is the mobile impurity concentration
- μ is the mobility
- E is the electric field
- D_A is the diffusivity

The Einstein relation relates mobility and diffusivity through the expression:

$$D = \frac{kT}{q} \mu$$

Diffusion models (3)

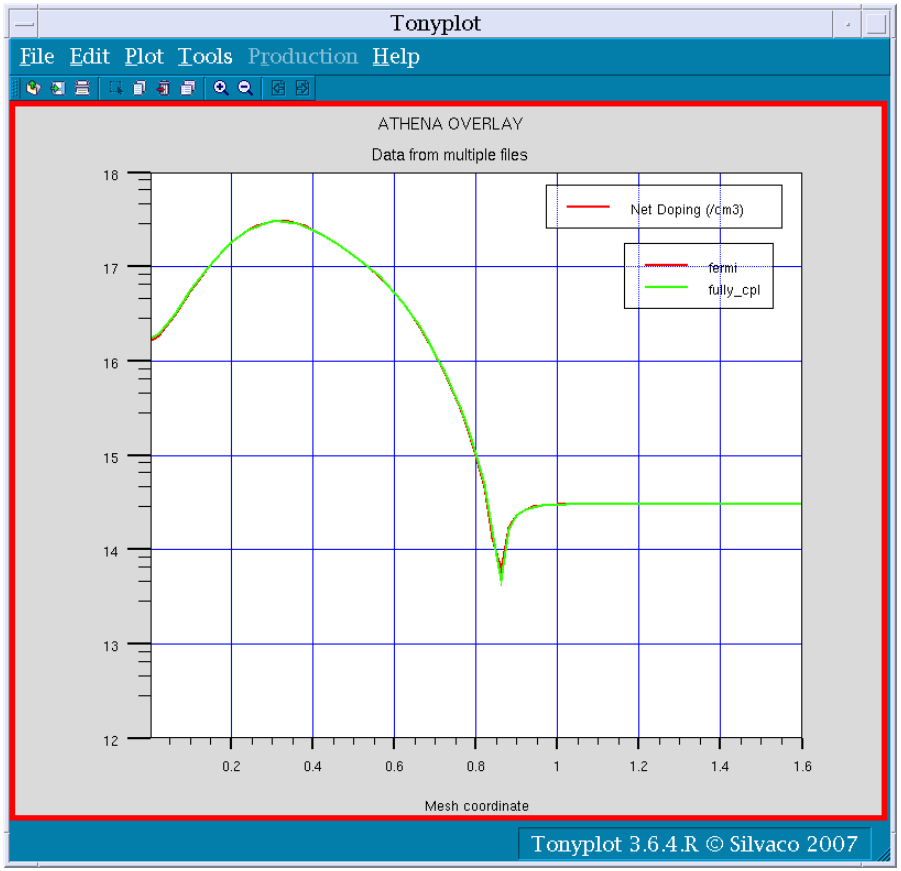
The main differences between athena diffusion models are the way point defects are represented. The selection of which model to use depends upon the existence or the generation of **point defects** during the diffusion process and the dopant concentrations within the silicon.

Model	Syntax	Assumption	Recommendation
Fermi (default)	*fermi*	**Defects in equilibrium**.	- Low concentration (less than1E20 cm^{-3}) - Inert ambient - Low execution time
Two dimensional	*two.dim*	**Transient defect diffusion**. Dopant diffusion influenced by point defects diffusion. Point defects diffusion is independent of dopant diffusion.	- Oxidation Enhanced Diffusion - Implant dose lower than 1E13 cm^{-2}
Fully coupled	*full.cpl*	**Two-way interaction** between dopants diffusion and point defects diffusion.	- Implant dose greater than 1E13 cm^{-2} - Co-diffusion (Emitter Push Effect) - Transient Enhanced Diffusion - RTA - High execution time

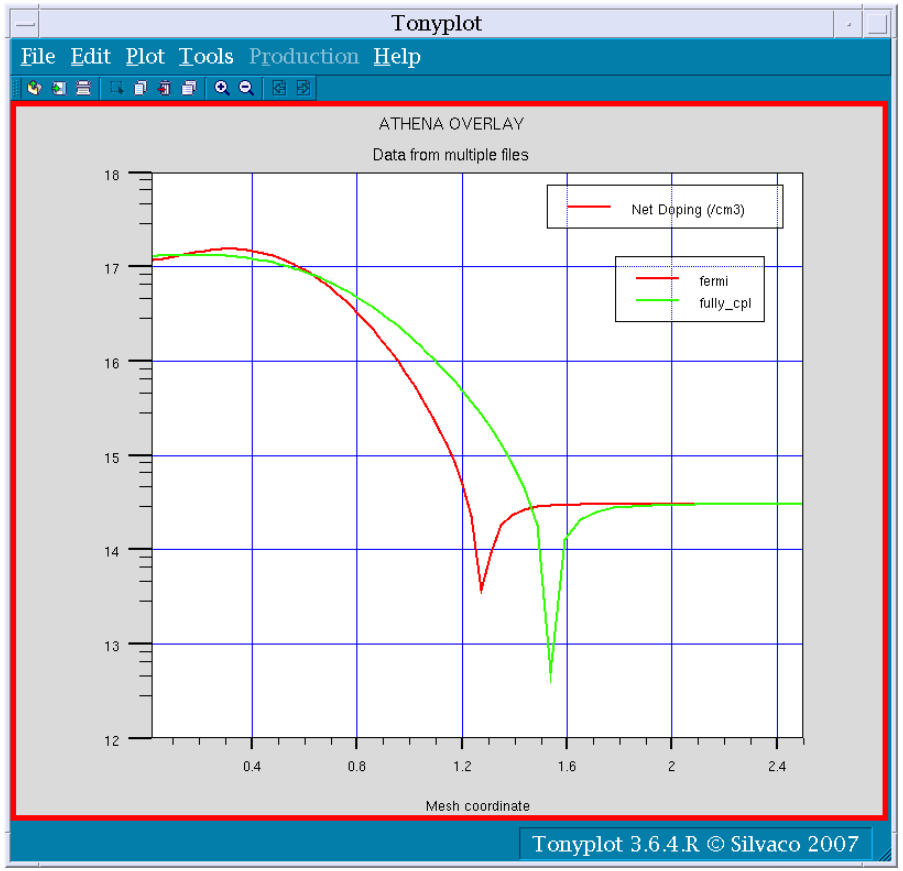
Diffusion models (4)

Make sure that the correct process models are used in the process flow!

diffusion temp=1100 time=30 **f.O2=0.08**



diffusion temp=1100 time=30 **f.O2=8.0**



fermi **fully coupled**

Question 6

To simulate a diffusion step, in oxidizing ambient after a high dose implant, the diffusion model to set is:

a) Fermi or Two Dimensional

b) Two Dimensional or Fully Coupled

c) Fully Coupled

Oxidation models (1)

The two-dimensional oxidation model is based on the ***linear-parabolic theory of Deal and Grove***. Silicon oxidation is modeled by considering the following three processes:

- Oxidant is transported from the ambient gas into the SiO_2 layer at the gas/SiO_2 interface.
- Oxidant is transported across the SiO_2 layer until reaching the Si/SiO_2 interface.
- Oxidant, arriving at the Si/SiO_2 interface, reacts with silicon to form a new layer of SiO_2.

The ***transport of oxidant*** across the gas/SiO2 interface is given by:

$$F = h(C^* - C_0)n_0$$

where:

- h is the gas-phase mass-transport coefficient.
- C^* is the equilibrium oxidant concentration in SiO_2.
- C_0 is the oxidant concentration in SiO_2 at the gas/SiO_2 interface.
- n_0 is a unit vector normal to the gas/SiO_2 interface pointing toward the silicon layer.

Oxidation models (2)

Silicon thermal oxidation is modeled when a DIFFUSION statement contains a **dryo2**, **weto2**, **f.o2**, or **f.h2o** parameter.

Model	Syntax	Assumption	Recommendation
Compress (default)	*compress*	Non-planar with linear flow.	Recommended for simulations of planar and non-planar structures, where stress effects play a minor role in determining the oxide shape.
Viscous	*viscous*	Non-planar with non linear flow.	When **stress effects** are important (e.g. birds beak with thick Si_3N_4). Execution time is higher.

The **grid.oxide** parameter in the METHOD statement (default is 0.1um) controls the number of grid layers added during the oxidation use

Model setting

Diffusion and oxidation models can be specified in the METHOD statement. In the Diffuse Menu, the Models field appears only when the corresponding check box is selected.