

1 Simulation tokens

This is an example file to describe all the features implemented in the current version (2001.05.08) of the **Ion Implantation In Semiconductors** program. The introduction of parameters is very simple. You must only write the correct (case sensitive) keyword in the input file and the values assigned to. The quantities shown with [] are used by default if the keyword does not appear. If some keyword appears twice or more times in the file, the program take the last value assigned to.

1.1 Atom definition

- Atom B 5 11.000 519.0
Atom Si 14 28.086 519.0
Atom O 8 15.994 519.0

Define the atoms involved in the problem. The order is important for next keywords (XTal, AtomP, etc.). The syntax is:

Atom Name(up to 2 chars) AtomicNumber AtomicMass(in uma) DebyeTemp

1.2 Layer definition

- Amorphous 2
[0]. The layer can be crystalline(0), polycrystalline(1) or amorphous(2).
- LatticeParameter 4.91304 4.91304 5.40463
[5.431 5.431 5.431]. Define the lattice parameters (a, b, c) measured in Å.
- Angles 90.0 90.0 60.0
[90 90 90]. Define the angles of the unit cell (α, β, γ). In degrees.
- XTal 2 1 0.3333 -0.4650 -0.4650 15
XTal 2 1 0.0000 0.0000 0.4650 15
XTal 2 1 0.6666 0.4650 0.0000 15
XTal 3 1 0.1200 0.2720 0.4150 15
XTal 3 1 0.4533 -0.4150 -0.1430 15
XTal 3 1 0.7866 0.1430 -0.2720 15
XTal 3 1 -0.1200 -0.2720 0.1430 15
XTal 3 1 0.5467 0.4150 0.2720 15
XTal 3 1 0.2133 -0.1430 -0.4150 15

Define each lattice site of the unit cell. Syntax:

XTtal NAtom Type Xpos Ypos Zpos BindingEnergy

where NAtom is the index of the atom (i.e.: 2=Si, 3=O) as you have introduced before. Type is the centered type. You can choose from: (1) primitive, (2) body centered, (3) A end centered, (4) B end centered, (5) C end centered, (6) face centered. Xpos Ypos

Zpos are the relative coordinates measured in lattice parameter units referred to the unit cell origin. BindingEnergy is the energy needed to move out an atom from his lattice site (in eV).

- XTal2 3 2 0.4 1 0.2133 -0.1430 -0.4150 15 10

Define each lattice site of the unit cell when alloys targets. Syntax:

```
XTtal2 NAtom1 NAtom2 Fraction1 Type Xpos Ypos Zpos BindingE1 BindingE2
```

where NAtom1 and NAtom2 are the indexes of the atoms (i.e.: 2=Si, 3=O) as you have introduced before. Fraction is the percentage/100 of the first atom. Type is the centered type. You can choose from: (1) primitive, (2) body centered, (3) A end centered, (4) B end centered, (5) C end centered, (6) face centered. Xpos Ypos Zpos are the relative coordinates measured in lattice parameter units referred to the unit cell origin. BindingE1 and BindingE2 are the energies needed to move out every atom from its lattice sites (in eV).

- XMin 0
[0]. X origin of the layer measured in Å.
- XMax 15.0
[1e9]. X limit of the layer measured in Å.
- EDTCreate 0
[0]. If you do not have a 3D electronic density for a particular target, you can select to create it (!=0) using for that the radial electronic densities of the atoms involved. These electronic densities must be in Nxx.den files (xx is the atomic number: boron(05), silicon(14)). The format of these files for each row is radius(Å) density(electron/Å³)
- EDTFile[EDT_SiO2]
File name of the 3D density. If you do not have the density and you wish to create it, the program put a proper name based in its chemical symbol. If you write here a file name the program overrides the file name calculated. If you have the density and the name matches the name generated by the program, you don't need to put any name.
- NextLayer
After the definition of one layer you can add more layers at the depth you wish. The keyword has no parameters.

```
// Define a layer of Si //
Amorphous 0
LatticeParameter 5.431 5.431 5.431
Angles 90.0 90.0 90.0
XTal 2 6 0.00 0.00 0.00 15
XTal 2 6 0.25 0.25 0.25 15
XMin 15.0 A
XMax 1e10
EDTCreate 0
EDTFile[ EDT_Si ]
```

1.3 Target definition

- **ABC 1 0 0**
[1 0 0]. Define the crystal orientation. Typically {100} or {110}.
- **FLAT 0 1 1**
[0 1 1]. Define the flat wafer orientation. Typically {011} or {001}.
- **Cut_Tha 3.5**
[0.0]. Define the cut angle of the wafer respect to the crystallographic orientation.
- **Cut_Phi 0.0**
[0.0]. Idem.
- **Therm 1**
[0]. Activate the thermal vibration model (!=0)
- **Temperature 300**
[300]. Defines the temperature of the target (in Kelvin). It is related to the thermal vibration model and with the Debye temperature defined in the atom definition section.

1.4 Simulation models

- **SpecificPotential 5 14 1**
Define the specific screening function for the potential used between Z_1 and Z_2 . You can select from:
 - 0: ZBl universal screening function.
 - 1: Specific screening function. Read from the file `ssfxxXX.dat` where `xx= Z_1` and `XX= Z_2` .
 - 2: Thomas-Fermi universal screening function.
 - 3: Molière universal screening function.
 - 4: Bohr universal screening function.
- **Stopping[Our]**
[Our]. Define the electronic stopping function used. You can select from:
 - None. No electronic stopping.
 - ZBL . Brandt-Kitagawa stopping model.
 - Our. Our Brandt-Kitagawa modified stopping model.
- **Ionizacion[ZBL]**
[ZBL]. Define the ionization curve used. You can select from:
 - ZBL. ZBL fit.
 - BK . Brandt-Kitagawa fit.
 - CGJ. Cai-Groenbech-Jensen fit.
 - MP . Mathar-Posselt fit.
- **RS0 2.0 0.0**
[1.85]. Define the r_s^0 parameter when Our *non-local* electronic stopping is used for each layer involved in the simulation. It must be end with 0.0
- **RecombinationFactor 0.06**
[0.06]. Define the f_{surv} parameter. Adimensional (Percentage/100).
- **AmorphizationDensity 4.99e21**
[4.99e21]. Define the N_α parameter. In at/cm^3

- **CutOffEnergy** 0.15
[0.15]. Define the E_{CutOff} parameter. In eV/Å³.
- **DisplacementEnergy** 15.0
[15.0]. Define the E_d parameter. In eV.
- **PreviousDamageFile** [Damage.old]
[(none)]. Define the previous damage file.
- **FullDoseOutput** 1
[0]. Define the temporal scaling when executing for the dose.

1.5 Projectile definition

- **AtomP** 1
[2]. Define the atom for the projectile (order number when the atoms were defined).
- **ENERGY** 2000
[200.0]. Define the implantation energy (in eV).
- **ENERGY_SPREAD** 0
[0.0].
- **ENERGY_SIGMA** 0
[0.0].
- **ENERGY_PERCENTAGE** 0
[0.0].
- **Dose** 1e14
[1e12]. Define the dose of the implantation.
- **Tha** 0
[0]. Polar angle (tilt) of implant direction (degrees)
- **Phi** 0
[0]. Azimutal angle (rotation) of implant direction (degrees)
- **WinA** 5.431
[5.431]. Define the implant window (in Å) (axe z or horizontal)
- **WinB** 5.431
[5.431]. Define the implant window (in Å) (axe y or vertical)
- **DivType** 0
[0]. Defines the statistical beam divergency model: (0) isotropically distributed, (1) obsolete, (2) non uniform cosine distribution.
- **Divergence** 0.5
[0.0]. Define the beam divergence (in degrees).

1.6 Implantation control

- **NumberOfImplants** 1000
[10]. Define the number of real atoms implanted.
- **LevelOfSimulation** 1
[1]. Indicates if the program must (= 1) follow only the primary ion (fast) or all the recoils.

- **MaxDepth** 15000
[1e10]. If the ion reach this depth then it is no longer followed. The ion has energy but we don't want to follow more. He is marked as ION-NOT-FOLLOWED but it appears in the final histogram.
- **MaxIterationsPerImplant** 100000
[10000]. The ion is no longer followed if this number of collisions or free flying steps are reached.
- **Seed1** 0
[1234].
Seed2 0
[5678]. Define the seeds for the Marsaglia random number generator used by the program.
- **InteractionRadius** 2.7155
[2.7155]. Defines the interaction radius used to search the targets to collide with (measured in Å)
- **SimultaneousDistance** 0.5
[0.5]. Defines the distance to considerate that the projectile go to collide simultaneously with two atoms or more (in Å).
- **SD2** 0.25
[0.25]. Defines the distance to considerate that the projectile go to collide simultaneously with two atoms or more (in Å). Second phase.
- **ThresholdEnergy** 10
[10]. Defines the threshold energy to follow a moving atom (in eV)

1.7 Rare event algorithm control

- **RareEvent** 0
[0]. Decades of precision (up to 6) with the rare event algorithm. Zero disables the rare event.
- **REShow** 0
[0]. Plot with *gnuplot* the splitting depths progress of the rare event algorithm. The quantities are stored in 'DEPTH' file. Zero disables this output.
- **REThreshold** 100
[100]. Number of real ions implanted to begin to recalculate the splitting depths for the rare event algorithm.
- **REInterval** 100
[100]. Number of real ions implanted to recalculate the splitting depths after reach the REThreshold.
- **REType** 1
[0]. Define the rare event behaviour. Uses depth (=0) or distance (!=0) as criterium.
- **pE** 0.25
[0.30]. Define the percentage of initial energy to activate the surface rare event .
- **pX** 0.5
[0.30]. Define the percentage of profile width to apply the surface rare event.

1.8 Graphic output control

- **HST 1**
[0]. Show (=1) the 1D implantation progress histogram.
- **HST2D 1**
[0]. Show (=1) the 2D implantation progress histogram.
- **HSTFile[As100]**
[Histo]. Define the histograms file name.
- **GPInit[set data style lines; set autoscale]**
[null]. Initializaton commands when showing the histogram progress with *gnuplot*. See *gnuplot* documentation. Up to 255 chars. Empty by default.
- **GPPlot[t "Current implantation"]**
[null]. Plotting commands that follows the command[plot "Histo"] when showing the histogram progress. See *gnuplot* documentation. Up to 255 chars. Empty by default.
- **PearsonIV 1**
[0]. Generate a Pearson IV distribution with the file name "G". The moments solved are also stored with the profile.

1.9 Multiple implants

- **NextSimulation**
The input file can describe several sequential implantations. This token defines a new one. The parameters that are take into account are:
 - AtomP
 - ENERGY
 - Tha
 - Phi
 - Divergency
 - NumberOfImplants
 - Dose
 - Temperature
 - RareEvent
 - RS0