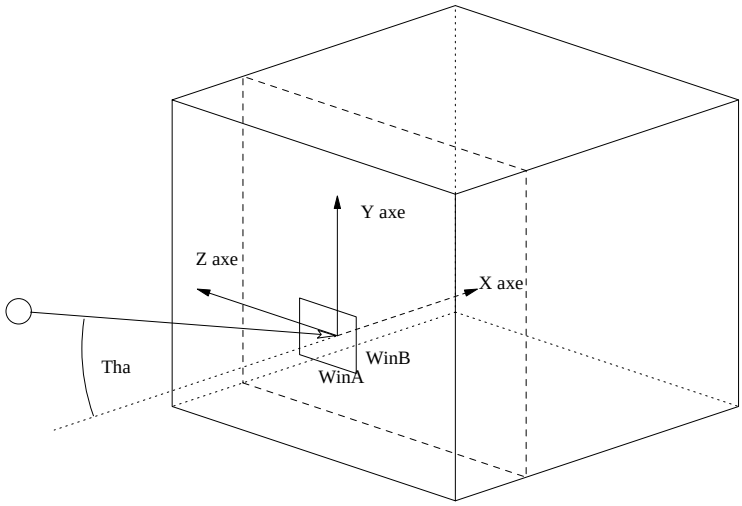
This help file describes all the features implemented in the current version (2003.10.13) of the IIS (Ion Implantation Simulator) program. The introduction of parameters is very simple. You must only write the correct -case sensitive- keyword in the input file and the values assigned to. The quantities shown with [] are 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.



Main tokens

ABC 1 0 0

[1 0 0] Define the X axis of simulation. It coincides with the crystal orientation.
In silicon:

<100> ⇒ ABC = 1 0 0, FLAT = 0 1 0
<110> ⇒ ABC = 1 1 0, FLAT = 0 0 1

FLAT 0 1 0

[0 1 0] Define the Y axis of simulation. It must be perpendicular to ABC, else program will stop.

WinA 5.431

Define the implant window (units Å)
[5.431] (axe z or horizontal)

WinB 5.431

Define the implant window (units Å)
[5.431] (axe y or vertical)

ImplantationArea 100.0

[100.0] Define the implantation area used by the 3D damage accumulation model (units Å^2)

Cut_Tha 0.0
Cut_Phi 0.0

Define the wafer cut error in tilt, tha, and rotation, phi (units: degrees)
[0.0] Tilt cut error of the wafer
[0.0] Rotation cut error of the wafer

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 the next keywords. The syntax is:

```
Atom_name(up_to_2_chars) atomic_number atomic_mass(in_uma) debye_temp(K)
```

The Debye temperature is for the thermal vibration model included. The atoms used as projectiles must be isotopes.

By default the program defines boron and silicon (in this order).

Target definition

Amorphous 0

[0] By default
(=0) Current layer is crystalline
(=1) Polycrystalline
(=2) Amorphous

XMin 0.0

[0.0] X origin of current layer (units: Å)

XMax 15.0

[1.0e9] X limit of current layer (units: Å)

LatticeParameter 5.431 5.431 5.431

[5.431 5.431 5.431]

Define the lattice parameters of the unit cell that reproduce the crystal (units: Å).

Angles 90.0 90.0 60.0

[90 90 90]

Define the angles of unit cell (alpha, beta, gamma). In degrees

```
XTal  2  1  0.3333  -0.465   -0.465    15 // Si
XTal  2  1  0.0      0.0      0.465    15 // Si
XTal  2  1  0.6666   0.465    0.0      15 // Si
XTal  3  1  0.12     0.272    0.415    15 // O
XTal  3  1  0.4533  -0.415   -0.143    15 // O
XTal  3  1  0.7866   0.143   -0.272    15 // O
XTal  3  1 -0.12    -0.272    0.143    15 // O
XTal  3  1  0.5467   0.415    0.272    15 // O
XTal  3  1  0.2133  -0.143   -0.415    15 // O
```

Define each lattice site of the unit cell. Syntax:

```
XTal n_atom type xpos ypos zpos binding_energy
```

where:
n_atom is the atom. It uses the introduction order number in the input file.

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.

binding_energy is the energy needed to destroy a link between atoms in this lattice site (units: eV).

```
Xtal2  3  2  1  0.2133  -0.143   -0.415  0.57  15  15
```

Define each lattice site of the unit cell. Syntax:

```
Xtal2 n_atom1 n_atom2 type xpos ypos zpos ratio binding_energy1 binding_energy2
```

where:

n_atom1, n_atom2 are the atoms that could appear in that lattice site. It uses the introduction order numbers of atoms in the input file.

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.

ratio is the number of times that n_atom1 statistically appears in that place. (1.0 - ratio) is number of times that n_atoms2 appears. It is useful for alloys like $In_x Ga_{1-x} As$

binding_energy1 binding_energy2 are the energies need to destroy a link between each atom and the crystal (units: eV).

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/Å^3))

EDTFile[EDT_SiO2]

[] Empty by default

(Text) File name of the 3D electron density. If you do not have the density and you wish to create it, the program can put a proper name based in its chemical symbol. If you write here a file name the program overrides the file name solved. 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 with no lateral limits, at the depth you wish. The keyword has no parameters.

```
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
XMax 1.0e10
EDTCreate 0
EDTFile[ EDT_Si ]
```

Implants

Projectiles 1 0

[2 0] Define the list of projectiles involved in that implantation (each number represents the order number of the atoms defined before). It is possible to simulate BF_2 implants, taking into account the damage generated by the F atom. The list must be ended with 0.

NumberOfImplants 1000

[10] Define the number of primary trajectories simulated for each set of projectiles

ENERGY 2000

[200.0] Define the implantation energy of each set of projectiles (units: eV). The energy is distributed between the projectiles according to their mass.

Miller 0

[=0] Select the direction of implant with the angles (Tha & Phi tokens)
(!=0) Select the direction of implant with the miller indexes (DIR token)

Tha 0

[0] Polar angle (tilt) of implant direction (unit: degrees)

Phi 0

[0] Azimuth angle (rotation) of implant direction (unit: degrees)

DIR 0 0 0

[0 0 0] Direction with miller indexes (dimensionless units). Used if Miller!=0

Divergence 1.5

[0.0] Define the divergence amplitude of the implant direction (unit: degrees)

Dose 1.0e13

[1e13]
Define the dose of the implantation (units: atom/cm^2). Used to calculate the histogram. The program does not take into account the dose rate.

Temperature 300

[300] Defines the temperature of the target (unit: Kelvin). It is related to the thermal vibration model and with the Debye temperature defined in the atom definition section. This token is take into account if the Therm token is activated

RareEvent 0

[=0] No rare event algorithm
(=D) Decades (up to 6) of precision with the rare event algorithm in order to reduce the statistical noise in the simulation speeding-up the simulation

RS0 1.85 0.0

[1.85 0.0] The only one fitting parameter for the electronic stopping model. Is a list of values, each one is for a layer of the target material. If there are more layers than values the last layers repeat the last value. It must be ended by 0.0

DoseSplitting Off

[Off] Does not uses the dose division algorithm. This algorithm is used to improve the statistical noise in high dose implants

DoseDistribution 1e13 1e14 1e15 0.0

[] If DoseSplitting is activated the simulator choose automatically a dose distribution, but you can override it by using this token. You write a list of doses to be simulated. The sum of that doses must not be greater than the Dose defined before. The last number 0.0 is needed to end the list and is replaced by the remainder dose (units: atom/cm^2).

Example:

Dose= 1e16
DoseDistribution = 1e13,1e14,1e15,0

The doses simulated sequentially will be: 1e13, 1e14, 1e15 and (1e16-1e15-1e14-1e13)

NextSimulation

This token indicates the simulator that must done another sequential implant simulation. You can repeat the above Implant tokens to define more sequential implants. The damage is accumulated from one to another.

Damage model

RecombinationFactor 0.06

[0.06] Is the survival factor of the defects generated at each time (units: dimensionless). By default uses the value fitted for Silicon.

KinchinPeaseConstant 0.8

[0.8] Is the Kinchin-Pease constant and must not be modified.

AmorphizationDensity 4.99e21

[0.1*4.99e22]

Is the amorphization density needed to consider the crystal amorphized (units: atom/cm^3). By default uses the value fitted for Silicon

DisplacementEnergy 15.0

[15.0] Is the displacement energy used in the Kinchin-Pease model (units: eV). You must adjust it for each target. By default uses the value extracted from experiments for Silicon.

CuttOffEnergy 0.15

[0.12] If you does not simulate the complete cascades (see LevelOfSimulation token) the simulator uses a correction to avoid that a volume of material becomes amorphized by only one impact. If the energy transferred is greater then the cut-off energy then the only energy transferred is the cut-off energy (units: eV/Å^3). If you simulates complete cascades this parameter is not used (more correct).

PreviousDamageFile[pepe]

[] By default is not used. Defines a previous damage file name.

Stopping models

Stopping[Our]

(text) Define the electronic stopping function used.
You can select from:

- None - No stopping
- ZBL - Brandt-Kittagawa stopping model
- Our - Our stopping model based on Cai-Groenbench model

Ionization[ZBL]

(text) Define the electronic ionization function used.
You can select from:

- ZBL - Ziegler-Biersack-Littmark ionization model
- BK - Brandt-Kittagawa ionization model
- CGJ - Cai-Groenbech-Jensen ionization model
- MP - Mattar-Posselt ionization model

SpecificPotential 5 14 1

Syntax: SpecificPotential Z1 Z2 Type

Z1 atomic number of the first atom

Z2 atomic number of the second atom

Type is the screening function used:

0 : Universal ZBL screening function.

Screening = 0.18179*exp(-3.2*X)+0.50986*exp(-0.9423*X)
+0.28018*exp(-0.4029*X)+0.02817*exp(-0.2016*X)

where X is the reduced distance = x/a_u

1 : Specific screening function

Simulator searches for a file named “ssfz1z2.dat” where z1 and z2 are the atomic numbers specified before. The file format will be:

Distance(Å) Screening Screening_Derivative

2 : Thomas-Fermi screening function

3 : Molière screening function
4 : Lenz-Jensen screening function
5 : Bohr screening function
6 : Specific screening function without potential derivative

Simulator searches for a file named "ssfz1z2.wopd" where z1 and z2 are the atomic numbers specified before. The file format will be:

Distance(Å) Screening

After run the simulator a file named "ssfz1z2.w" will contain also the potential derivative.

Advanced 1

LevelOfSimulation 1

(0) Follows all levels of projectiles (slow)
[1] The program only follows the primary ion trayectory (fast)

Randomize 1

(0) Assume initial positions give by POS keyword
[1] Assume random positions

Seed1 1234

[1234] Seed for the Marsaglia random number generator used by the program

Seed2 5678

[5678] Seed for the Marsaglia random number generator used by the program

POS 0 0 0

[0 0 0] Fixed initial position of each set of projectiles. If Randomize keyword is activated, this field is not taken into account

Advanced 2

SimultaneousDistance 0.5

[0.5] Defines the distance to considerate that the projectile go to collide simultaneously with two atoms or more (units: Å). Before collisions.

SD2 0.25

[0.25] Defines the distance to considerate that the projectile go to collide simultaneously with two atoms or more (units: Å). After collisions.

GhiLimit 0.1

[0.1] Defines the minimum distance in the direction of the projectile to search new targets to not collide two times with the same target atom (units: Å)

ThresholdEnergy 10

[10] Defines the threshold energy to follow a projectile (units: eV)

InteractionRadius 2.7155

[2.7155] Defines the interaction radius used to search the targets to collide with (units: Å)

MaxDepth 15000

[1e10] The ion is not longer followed if it reaches this depth. 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

[1e4] The ion is not longer followed if this number of collisions or free flying steps are reached.

Therm On

[On] Activate the thermal vibration model

EnergySpread 0

[0] The energy can vary from nominal energy following one of the following distributions:

0 : No dispersion

1 : Uniform distribution between

```
{ENERGY – EnergySigma/2, ENERGY + EnergySigma/2}
```

2 : Gaussian distribution using EnergySigma

EnergySigma 0.0

[0.0] Define the dispersion of the distribution defined above (units: eV)

EnergyPercentage 0.0

[0] If defined (not 0) the EnergySigma = ENERGY*EnergyPercentage/100

DivType 2

[1] Defines the statistical divergence model for the implant direction

(=0) isotropic distribution

(=1) non uniform cosine distribution (around azimuth angle)

REThreshold 100

[100] Number of trajectories simulated for each set of projectiles in order to recalculate the splitting depths for the rare event algorithm (with depth or distance)

REInterval 100

[100] Number of trajectories simulated to recalculate the splitting depths after reach the REThreshold

REType 0

[0] Type of rare event to use :

0 : Statistical noise reduction based on depth

1 : Statistical noise reduction based on distance

RareEvent 0

[0] Number of orders of magnitude of extra accuracy in the statistical noise reduction algorithm: not for surface rare event

pE 0.0

[0.0] Energy percentage (between 0.0 and 1.0) to activate surface rare event. By default is deactivated. A typical value could be 0.10

pX 0.0

[0.0] Depth percentage (between 0.0 and 1.0) to activate surface rare event. By default is deactivated. A typical value could be 0.05

Output tokens

Verbose Off

[Off] Display extra information.

Also saves to disk (Layer_XX.xyz) the crystallite used corresponding to each layer in .xyz format readable with Xmol-like programs (xmol, chime, rasmol, raswin, etc.)

PearsonIV Off

[Off] Saves to disk a Pearson IV profile fitted to simulated profile if possible. The file name will be "pearsonIV_xx", where xx is the number of projectile. The format is

distance (nm), conc. Gaussian distrib. (at/cm^2), concentration PearsonIV distribution (at/cm^2)

and includes the solved moments. Example:

```
#  Pearson IV moments:
# Mean range m1 = 272.536
# Straggle   m2 = 201.059
# Skewness   m3 = 1.02545
```

```
# Kurtosis   m4 = 4.11697
# Cannot generate a Pearson IV
```

HSTFile[profile]

[Histo1D.xx_yy] Filename for the 1D doping profile. The simulator adds to the filename "xx_yy" where xx is the implant number and yy is the projectile number (order of implantation)

ShowHisto1D On

[Off] Shows the 1D doping profile in runtime in a gnuplot window (only unix systems) . In Windows systems a file named "gnuplot0.dat" will contain the gnuplot commands to plot the file

GPInit[set data style lines; set auto scale]

(Text) Initialisation commands when showing the doping profile progress with gnuplot. See gnuplot documentation. Up to 255 chars. Empty by default.

GPPlot[t "Current implantation"]

(Text) Plotting commands that follow the command{ plot "Histo1D." } when showing the doping histogram progress. See gnuplot documentation. Up to 255 chars. Empty by default.

ShowDamage On

[Off] Shows the 1D damage profile in runtime in a gnuplot window (only unix systems) . In Windows systems a file named "gnuplot2.dat" will contain the gnuplot commands to plot the file

GPInitDamage[set data style lines; set auto scale]

(Text) Initialisation commands when showing the damage profile progress with gnuplot. See gnuplot documentation. Up to 255 chars. Empty by default.

GPPlotDamage[t "This work", "B_Si.rbs"t "Experimental RBS"]

(Text) Plotting commands that follow the command{ plot "Histo1D." } when showing the damage histogram progress. See gnuplot documentation. Up to 255 chars. Empty by default.

FullDoseOutput On

[Off] Show the doping profile scaled or not to the total dose at runtime

REShow Off

[Off] Plot splitting depths . The data is stored in 'RE_Depths.xx' file, where xx is the number of projectile

ASCII Off

[Off] Shows 3D profiles in ASCII format

Example 1

Boron into crystalline silicon with an amorphous layer of silicon oxide of 15 Å width at room temperature. The crystal orientation for Silicon is {100} for the depth axis and the ion beam is rotated 30º and tilted 7º and has an energy of 15000 eV. The divergence of the beam is 0.5º. The dose is 1e14 atom/cm^2

Input filename: B_Si.in

```
 RS0 1.85 1.85 0.0 // the only one fitting parameter for silicon
 Divergency 0.5
 RareEvent 2 // two extra orders of accuracy

 ENERGY 15000 eV
 Dose 1e14
 NumberOfImplants 5000

 ABC 1 0 0
 Tha 7 degrees (tilt)
 Phi 0 degrees (rotation)

 Temperature 300 kelvin

 Atom B   5 11.000  519.0 // atom 1
 Atom Si 14 28.086  519.0 // atom 2
 Atom O   8 15.994  519.0 // atom 3
 Projectiles 1 0

// SiO2
 LatticeParameter   4.91304   4.91304   5.40463
 Angles            90.0      90.0    60.0
 XTal  2  1  0.3333  -0.465   -0.465  15  // Si
 XTal  2  1  0.0      0.0      0.465  15  // Si
 XTal  2  1  0.6666   0.465    0.0    15  // Si
 XTal  3  1  0.12     0.272    0.415  15  // O
 XTal  3  1  0.4533  -0.415   -0.143  15  // O
 XTal  3  1  0.7866   0.143   -0.272  15  // O
 XTal  3  1 -0.12    -0.272    0.143  15  // O
 XTal  3  1  0.5467   0.415    0.272  15  // O
 XTal  3  1  0.2133  -0.143   -0.415  15  // O
 Amorphous 2 // amorphous
 XMin 0 A
 XMax 15.0 A

 NextLayer

// Si <100>
 XTal 2 6 0.00 0.00 0.00 15  // Si
 XTal 2 6 0.25 0.25 0.25 15  // Si
 Amorphous 0 // crystalline
 XMin 15.0 A
```

Output filenames:
All of this in the DB_Si.in directory

```
Parameters.out
Histo1D.01_01
Ion.01.histo3D.bin
Amorph1D.dat
```

Parameters.out. This file includes all the parameters used by the simulator. You can use this file to known if the simulator has understood the input file and to known the rest of parameters used. Some parameters are twice or more times.

```
               Projectiles =          1,0,0,0,0,0,0,0,0,0,
                   ENERGY =      500.0
                      DIR =         (     1.000,     0.000,     0.000 )
                   Miller =          0
                      Tha =      7.000
                      Phi =      0.000
                Divergence =      0.000
         NumberOfImplants =       1000
                     Dose =  1.000e+13
              Temperature =      300.0
                RareEvent =          2
                      RS0 =      1.850,1.850,1.850,1.850,1.850,
            NextSimulation =
Implanted atoms 1, 0, 0, 0, 0, 0, 0, 0, 0, 0
Energy         = 500.0 eV
Tha, Phi       = 7.000, 0.000Divergency     = 0.000
Implants       = 1000        Dose           = 1.000e+13at/cm^2
DoseSplitting  Off
Temperature    = 300.0       Rare Event     = 2
RS0            = 1.850,1.850,1.850,1.850,1.850,0.0

             EnergySpread =          0
              EnergySigma =      0.000
          EnergyPercentage =      0.000
                      POS =         (     0.000,     0.000,     0.000 )
                  DivType =          1
         InteractionRadius =      2.716
           ThresholdEnergy =      10.00
                  GhiLimit =     0.1000
     SimultaneousDistance =     0.5000
                      SD2 =     0.2500
                  Verbose =        Off
                    Seed1 =       1234
                    Seed2 =       5678
                Randomize =          1
                      ABC =         (     1.000,     0.000,     0.000 )
                     FLAT =         (     0.000,     1.000,     0.000 )
                  Cut_Tha =      0.000
                  Cut_Phi =      0.000
                     WinA =      5.431
                     WinB =      5.431
                    Therm =         On
  MaxIterationsPerImplant =     100000
                 MaxDepth =  1.000e+10
         LevelOfSimulation =          1
                     Atom =
[B]    W =     11.00 amu, Z =   5, TDebye = 519.0 K, TAmp =     0.1262 A
[Si]   W =     28.09 amu, Z =  14, TDebye = 519.0 K, TAmp =    0.07897 A
[O]    W =     15.99 amu, Z =   8, TDebye = 519.0 K, TAmp =     0.1047 A


        SpecificPotential =
                Amorphous =          0
         LatticeParameter =         (     5.431,     5.431,     5.431 )
                   Angles =         (     90.00,     90.00,     90.00 )
                     XTal =
    Atom 2 : FACE CENTERED(     0.000,     0.000,     0.000 ) 15.00 eV
    Atom 2 : FACE CENTERED(    0.2500,    0.2500,    0.2500 ) 15.00 eV

                     XMin =      15.00
                     XMax =  1.000e+09
               EDTFile[ =
              EDTCreate =          0
              NextLayer =

==> AMORPHOUS layer ( 0.000 to 15.00 ) A
    LatticeParameter (     4.913,     4.913,     5.405 ) A
    Angles           (     90.00,     90.00,     60.00 )
    EDTFile          ' ' (old)

    Atom 2 : PRIMITIVE(    0.3333,   -0.4650,   -0.4650 ) 15.00 eV
    Atom 2 : PRIMITIVE(     0.000,     0.000,    0.4650 ) 15.00 eV
    Atom 2 : PRIMITIVE(    0.6666,    0.4650,     0.000 ) 15.00 eV
    Atom 3 : PRIMITIVE(    0.1200,    0.2720,    0.4150 ) 15.00 eV
    Atom 3 : PRIMITIVE(    0.4533,   -0.4150,   -0.1430 ) 15.00 eV
    Atom 3 : PRIMITIVE(    0.7866,    0.1430,   -0.2720 ) 15.00 eV
    Atom 3 : PRIMITIVE(   -0.1200,   -0.2720,    0.1430 ) 15.00 eV
    Atom 3 : PRIMITIVE(    0.5467,    0.4150,    0.2720 ) 15.00 eV
    Atom 3 : PRIMITIVE(    0.2133,   -0.1430,   -0.4150 ) 15.00 eV

==> CRISTALLINE layer ( 15.00 to 1.000e+09 ) A
```

```
LatticeParameter (     5.431,     5.431,     5.431 ) A
Angles           (     90.00,     90.00,     90.00 )
EDTFile          ' ' (old)

Atom 2 : FACE CENTERED(     0.000,     0.000,     0.000 ) 15.00 eV
Atom 2 : FACE CENTERED(    0.2500,    0.2500,    0.2500 ) 15.00 eV

          REThreshold =        100
           REInterval =        100
               REShow =        Off
               REType =          0
                   pE =      0.000
                   pX =      0.000
            PearsonIV =        Off
          ShowHisto1D =        Off
           ShowDamage =        Off
       FullDoseOutput =         On
             HSTFile[ =          Histo1D.
              GPInit[ =
              GPPlot[ =          t "This work"
          InitDamage[ =
          PlotDamage[ =          t "This work"
            Stopping[ =          Our
          Ionization[ =          ZBL
                PAUSE =          0
  RecombinationFactor =    0.06000
 KinchinPeaseConstant =     0.8000
 AmorphizationDensity =  4.990e+21
         CutOffEnergy =     0.1500
   DisplacementEnergy =      15.00
  PreviousDamageFile[ =
        DoseSplitting =        Off
    DoseDistribution =      0.000,0.000,0.000,0.000,0.000,
    ImplantationArea =      100.0
                ASCII =        Off
```

Histo1D.01_01. This file is the doping profile obtained by the first implant and the first projectile of that implant.. The format is

```
# 1000 10000
100    102.302
```

Example 2

Boron into