Crystal-TRIM (04/1D - last revision May 2004)

developed by Matthias Posselt [1) 2)]

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Other versions of Crystal-TRIM were part of the process simulators $\mathrm{TESIM}_{-\mathrm{ISE}}$ $\mathrm{DIOS}_{-\mathrm{ISE}}$**, and** $\mathrm{FLOOPS}_{-\mathrm{ISE}}$ **which were distributed by ISE Integrated Systems Engineering AG Zürich, Switzerland. Now some of these simulators are part of the TCAD software of Synopsys**$^{(R)}$**.**

GENERAL REMARKS

Crystal-TRIM simulates ion implantation into single-crystalline silicon, germanium and into diamond with ≤ 10 amorphous overlayers of arbitrary composition (with ≤ 3 components). Not only atomic ions but also molecular ions (with ≤ 3 components) can be considered. Dynamic simulation of damage accumulation in the single-crystalline substrate, including the formation of amorphous layers, is possible. Note, that the code has not been tested yet for germanium and diamond. The parameter values given below are only valid for Si substrates.

The physical background of Crystal-TRIM has been described in the papers given in the reference list [1)] below. The main applications of the code have been investigations on channeling effects and defect evolution during ion bombardment.

The present version can be used to calculate as-implanted range and damage distributions as a function of depth. In this case, an efficient splitting procedure [2)] can be employed in order to enhance the statistical accuracy of the simulation results without considerable increase of computing time. It is particularly useful if so-called channeling tails are of interest.

Two-dimensional profiles can be also simulated if damage accumulation during ion bombardment does not play a role.

The following files are necessary for all applications of Crystal-TRIM:
scoef1.dat, scoef2.dat, xtru04.exe, xtr041.exe, prof1z.exe, prof2z.exe
Do not delete these files!

Improvements compared to version 98/1D:

Introduction of germanium and diamond as single-crystalline substrates.

Parameters Cel and Cel110 used in the semiempirical formula for the local electronic energy loss (modified Oen-Robinson model)

The default value of these parameters is 1. In the following tables some cases are given where other values are recommended.

Boron (in B^+ or BF_2^+)

incidence energy (keV)	**Cel110**	**Cel**
0.2-0.5		2.2-2.0
1.		1.8
2.-4.		1.6
5.		1.5
8.		1.35
10.		1.32
15.		1.25
20.		1.2
30.		1.1
600.	0.77	0.9
700.		0.9

Fluorine (in BF_2^+)

incidence energy (keV)	**Cel110**	**Cel**
6.		1.8
14.		1.5
25.		1.4
52.		1.3

Phosphorus

incidence energy (keV)	Cel110	Cel
30.		1.5
100.	0.97	1.45
200.	0.93	1.37
500.	0.84	1.12
1000.	0.77	1.05

Arsenic

incidence energy (keV)	Cel110	Cel
15.		2.
50.		1.57
80.		1.46
180.		1.3

Phenomenological models of damage accumulation during ion bombardment
Model numbers: 1, 2, 3, 4, 5, 6

The modeling of damage accumulation has been improved several times. In the following the notation of the models and the meaning of the parameters used in the present version of Crystal-TRIM are briefly described. These are the same as in version 96/1D.

1, 2, 3: point defect accumulation (interstitials and vacancies)

Interstitial sites:
tetrahedral interstitial sites, or interstitial sites randomly distributed within a cube of volume l^3 where l is the mean atomic distance in silicon

1: parameter cacc

cacc = 1.: no in-situ annealing of the atomic displacements created during ion impact,

cacc $\neq$ 1.: (100*cacc)% of created damage remains after a single (pseudo-)ion impact

2: parameters cacc and ccrit

cacc as described,

ccrit = 1.: equivalent to **1**

ccrit $\leq$ 1.: damage saturation at a damage concentration of (100*ccrit)%

3: parameters cacc and ccrit

cacc as described,

ccrit = 1.: equivalent to 1

ccrit $\leq$ 1.: full amorphization above a critical damage concentration of (100*ccrit)%

4, 5, 6: accumulation of amorphous pockets

4: parameter cacc

cacc = 1.: no in-situ annealing

cacc $\neq$ 1.: (100*cacc)% of created damage remains after a single (pseudo-)ion impact

5: parameters cacc and ccrit

cacc as described,

ccrit = 1.: equivalent to **4**

ccrit $\leq$ 1.: damage saturation at a damage concentration of (100*ccrit)%

6: parameters cacc and ccrit

cacc as described,

ccrit = 1.: equivalent to **4**

ccrit $\leq$ 1.: full amorphization above a critical damage concentration of (100*ccrit)%

Recent investigations showed that model 6 is the most realistic damage accumulation model in many applications. The following table gives recommended values of the parameters cacc and ccrit for typical examples.

ion	**cacc**	**ccrit**	
B^+	0.1	≥ 0.5	**but: cf. Ref. [22]**
BF_2^+	0.17	0.1	
P^+	0.2	0.1	
As^+, In^+,Sb^+	0.3	0.05	**but: cf. Ref. [22]**

Splitting procedure [2)]

The default splitting procedure is always recommended. A considerable increase of computational efficiency is obtained: The ratio between the CPU-time of a simulation without the default splitting algorithm and the time of a calculation using this method is about 5 to 10, if the same statistical accuracy is required for the results of both simulations. A measure of the statistical accuracy of depth profiles is the number of independent (pseudo)projectiles ISIGDEPTH which contribute to particle trajectories in a certain depth SIGDEPTH. The value of ISIGDEPTH (usually between 5 and 20) must be defined by the user during the input dialog, SIGDEPTH is determined at the end of simulations and is given in the name.**OUT file (see pages 5,6,7). The value of SIGDEPTH is also important in order to estimate the statistical significance of long "channeling tails" in the simulated depth profiles.**

Note, that in cases where the default splitting procedure is used in connection with damage accumulation model 3 or 6, the number of (pseudo)projectile histories really followed in the simulations will be generally (up to 1.5 times) higher than that number defined by the user during the input dialog (see page 5) and given in the name.**OUT** file and by the on-line informations during the run.

HOW TO USE Crystal-TRIM ?

Step 1:

Dialog using the program **xtru04.exe**

All input parameters are asked for during the dialog.

command: xtru04.exe
(creates all input-files, gives the output-files their names, **does not** the simulation)

2 different types of runs ("run" = simulation) can be prepared:

type 1:
new run

type 2:
rerun, i.e. intermediate results (mainly profile data) of a previous run are used in a subsequent run - a way in order to improve the statistical accuracy of the simulations by using results of previous runs)
(files: name**.IN**, name**.DAT**, name**.ST must** exist),
in a rerun the input data are the same as in the previous run
(exception: number of particles to be simulated in the rerun)

Which **input-files** are created by **xtru04.exe** ?

type	**example**
name **.IN**	b15s**.IN**
name **.DAT**	b15s**.DAT**

Note that name consists of 4 ASCII characters exactly!

Which **names** of output-files are created by **xtru04.exe** ?

description	**type**	**example**
output-file with a "listing" of the results	name **.OUT**	b15s**.OUT**
output-file with the table of all 1d profiles (depth profile of the atomic component n of the (possibly) molecular ion ($1 \leq n \leq 3$), and energy deposition and damage profiles, created by **all** components of the molecular ion)	name **.1D**n	b15s**.1D**1
output-file with the table of all 2d profiles (range, energy deposition and damage profiles created by **all** components of the (possibly) molecular ion)	name **.2D**	b15s**.2D**
file with intermediate results which can be used in a rerun	name **.ST**	b15s**.ST**

Step 2:

Run of the simulation code **xtr041.exe**

command: xtr041.exe < name**.IN**
(**does** the simulation)

During the run some informations about the status of calculations appear on the screen.

Results:

description	**type**	**example**
output-file with a "listing" of the results	name **.OUT**	b15s**.OUT**
output-file with the table of all 1d profiles (depth profile of the atomic component n of the (possibly) molecular ion ($1 \leq n \leq 3$), and energy deposition and damage profiles, created by **all** components of the molecular ion)	name **.1D**n	b15s**.1D**1
output-file with the table of all 2d profiles (range, energy deposition and damage profiles created by **all** components of the (possibly) molecular ion)	name **.2D**	b15s**.2D**
file with intermediate results which can be used in a rerun	name **.ST**	b15s**.ST**

After Step 2:

$\Longrightarrow$ **Step 1** for a rerun or $\Longrightarrow$ **Step 3** for preparation of diagrams

Step 3:

Preparation of diagrams

1d

command: **prof1z.exe**

input-file:
file containing the tables of all 1d profiles (example: b15s**.1D**1)
output-file:
new file which contains one selected 1d profile:
range profile, profile of nuclear or electronic energy deposition, damage concentration profile, depth distribution of the damage probability
Note that the latter depth distribution is needed in subsequent simulations of ion implantation into a predamaged target!

form of output-files:
depth coordinate (nanometer) - first column
value - second column
The dimension of " value" is cm^{-3} or eV/target atom,

The output file created can be used to get a histogram,
e.g. by using a PC graphics software tool.

Attention:
Since in many cases a logarithmic plot will be used for "value", in **prof1z.exe** the value "0" is replaced by the minimum, non-zero value of "value". This can lead to some confusion if results show poor statistics.

2d

command: **prof2z.exe**

input-file:
file containing the tables of all 2d profiles (example: b15s**.2D**)
output-file:
new file which contains one selected 2d profile
(range, or nuclear energy deposition, or electronic energy deposition, or displacements)
form of output-files:
depth coordinate (Å) -first column
lateral coordinate(Å) - second column
value - third column

The dimension of "value" is $Å^{-2}$ or $eVÅ^{-2}$.

The output-file created can be used to get a 3d histogram,
e.g. by using a PC graphics software tool.

Note:
In Crystal-TRIM the 2d profiles are calculated for a "one-particle line source"
at the target surface.

1) References:

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[2] M. Posselt: Crystal-TRIM and its application to investigations on channeling effects in ion implantation, Radiation Effects and Defects in Solids **130/131** (1994) 87.

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2) Acknowledgements:

The data file **scoef1.dat** corresponds to the data file scoef.dat published in [*a*]. The data file **scoef2.dat** corresponds to the corrected scoef.dat file used in 1989 in the standard TRIM code [*a*, *b*]. In the above references the file **scoef1.dat** was used. For common applications of Crystal-TRIM the differences between **scoef1.dat** and **scoef2.dat** are not important. In the program Crystal-TRIM the description of the nuclear scattering, the registration of physical quantities (e.g. stopped ions, displaced atoms, nuclear and electronic energy deposition) and the treatment of the motion of a projectiles in the amorphous surface layer are similar to the corresponding procedures used in the standard TRIM program [*a*, *b*].

[*a*] J.F. Ziegler, J.P. Biersack, U. Littmark: The Stopping and Range of Ions in Solids, Pergamon Press, New York, 1985.
[*b*] J.P. Biersack, L.G. Haggmark, Nuclear Instruments and Methods **174** (1980) 257.

The splitting procedure was developed by Bruno Schmidt who was PhD student in our group.