

Crystal-TRIM

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The present version of Crystal-TRIM is result of the last comprehensive revision in May 2004.

Other versions of Crystal-TRIM were part of the process simulators TESIM-ISE, DIOS-ISE, and FLOOPS-ISE, which were formerly distributed by ISE Integrated System Engineering AG Zürich, Switzerland. Now some of these simulators are part of the TCAD software of Synopsys®.

Crystal-TRIM for Linux and Windows

All executables must be started from the “command line”.

Crystal-TRIM was developed and mainly used on Linux and other Unix systems where upper and lower case letters are recognized as different. Under Windows the command line in the MSDOS mode must be used (“execute”, with input “cmd”). Note that in MSDOS there is no difference between upper and lower case. This should be considered if the names of input and output files are chosen.

1. General Remarks

Crystal-TRIM simulates ion implantation into single-crystalline silicon, germanium and into diamond with ≤ 10 amorphous top-layers 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. On the other hand, the composition of the target does not change during the simulation so that effects such as ion-beam synthesis, sputtering, and ion-beam-induced mixing of the target during high dose (or high fluence) implantation cannot be described. Note, that the code was not carefully tested for germanium and diamond. The special parameter values given below are only valid for case with a single-crystalline Si (c-Si) substrate.

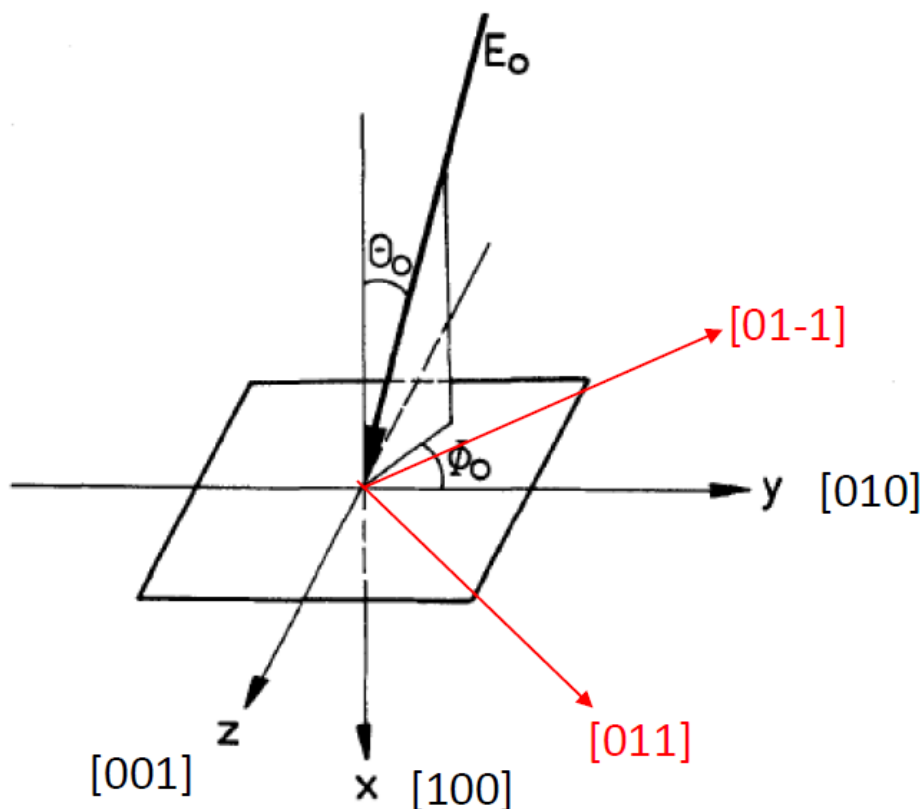
The physical background of Crystal-TRIM is described in the papers given in the reference list¹⁾ below. Main applications of the code were

investigations on channeling effects and the influence of damage accumulation during ion bombardment on channeling.

The present version can be used to calculate as-implanted range and damage distributions as a function of depth. An efficient splitting procedure (see 1.3) can be employed in order to enhance the statistical accuracy of the simulation results without a considerable increase of computing time. Splitting is particularly useful if so-called low-concentration channeling tails are of interest since these determine the depth of the p-n junction.

Note that in Crystal-TRIM the ion energy is always the kinetic energy of the ion upon impact, i.e. the ion charge is not an input data. The number of ion (or projectile) histories used in the simulation can be freely chosen. It should be noticed that each projectile represents a certain ion dose. In the following, the terms "ion" and "projectile" are used as synonyms, and this may be also a molecule ion or projectile.

The following geometry is implemented in Crystal-TRIM: The tilt angle is defined with respect to the surface normal. The figure shows the case of a (100) substrate where the surface normal is parallel to the [100] direction. The rotation or twist angle is defined with respect to the [010] direction. Note that in practice the twist angle is often (not in all cases!) given with respect to the main wafer flat, which is parallel to [011] or [01-1]. Then, the absolute value of the difference between this angle and 45° gives the rotation angle to be used in Crystal-TRIM.



1.1 Crystal-TRIM files

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

The files scoef1.dat, scoef2.dat contain general data from different commonly accessible databases as well as the ZBL electronic stopping parameters provided by two versions of the TRIM code²⁾. In most of the previous Crystal-TRIM calculations (see reference list¹⁾) the file scoef1.dat was used.

1.2 Semi-empirical parameters used in the code

In Crystal-TRIM, few semi-empirical parameters are used. Their values were obtained by comparing simulation results with experimental depth profiles, which were preferentially measured by SIMS.

1.2.1 Parameters of the electronic stopping models

If the ion dose is low so that damage accumulation during implantation is negligible (e.g. below some 10^{13} cm⁻² in P implantation into c-Si), only parameters determining the electronic energy loss of the ion must be considered:

clambda: Determines the “random peak” of the ion range (depth) profile, i.e. is not related to channeling. This peak would be also found if the material were amorphous. The value of clambda is around 1 and is provided by the scoef*.dat files. This parameter is part of the ZBL electronic stopping power model. In general, higher/lower values yield a smaller/larger depth of the “random peak”.

Cel and Cel110: Determine the channeling in the [110] direction (Cel110) and in all other directions (Cel). The default and implemented value of the two parameters is 1. In general, values higher/lower than 1 lead to more/less channeling. Since in practice [110] channeling implantations (or in crystallographic equivalent <110> directions, such as [011] etc.) are uncommon, only Cel is of real importance. The parameters Cel110 and Cel are part of the modified Oen-Robinson model, which describes the dependence of the electronic stopping of a projectile on the distance from a target atom.

Recommended values of Cel (and Cel110) if they differ from 1:

Boron (or B atom in BF₂)

Initial 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 (F atom in BF₂)

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

Phosphorus

Initial 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

Initial energy (keV)	Cel110	Cel
15.		2.0
50.		1.57
80.		1.46
180.		1.3

1.2.2 Parameters of the damage accumulation models

At higher ion doses damage accumulation during ion bombardment must be taken into account since this effect leads to increasing dechanneling. That means that the concentration of the channeling part of the depth profile does not increase further with dose, in contrast to the random part. Different phenomenological models for damage accumulation were developed within the framework of Crystal-TRIM, see also the publications in the reference list¹⁾ below. In these models, the increase of damage in each depth interval is registered and converted into the probability that a subsequent projectile meets vacancies/self-interstitials or amorphous material (pockets) in the considered depth interval. Most successful were models considering accumulation of amorphous pockets, in particular model 6. It is recommended to use this, or model 5 if damage saturation takes place (e.g. at high temperature). However, in the following all available models are listed.

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

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

Model 1: parameter **cacc**

cacc = 1.: damage accumulation of each ion impact contributes to total damage

cacc ≠ 1.: only $(100 \cdot cacc)\%$ of the total damage remains before the next projectile impact

Model 2: parameters **cacc** and **ccrit**

cacc as described above,

ccrit = 1.: equivalent to model 1

ccrit ≤ 1.: saturation of total damage at a total damage level of $(100 \cdot ccrit)\%$

Model 3: parameters **cacc** and **ccrit**

cacc as described,

ccrit = 1.: equivalent to model 1

ccrit ≤ 1.: full amorphization above a critical total damage level of $(100 \cdot ccrit)\%$

Models 4, 5, 6: accumulation of amorphous pockets

Model 4: parameter **cacc**

cacc = 1.: damage accumulation of each ion impact contributes to total damage

cacc ≠ 1.: only $(100 \cdot cacc)\%$ of the total damage remains before the next projectile impact

Model 5: parameters **cacc** and **ccrit**

cacc as described,

ccrit = 1.: equivalent to 4

ccrit ≤ 1.: saturation of total damage at a total damage level of $(100 \cdot ccrit)\%$

Model 6: parameters **cacc** and **ccrit**

cacc as described,

ccrit = 1.: equivalent to 4

ccrit ≤ 1.: full amorphization above a critical total damage level of $(100 \cdot ccrit)\%$

The following table shows recommended values of the parameters **cacc** and **ccrit** for typical examples.

projectile (ion)	cacc	ccrit
B	0.1	≥0.5, but Ref. [22]
BF ₂	0.17	0.1
P	0.2	0.1
As, In, Sb	0.3	0.05, but Ref. [22]

Note that the BF₂ projectile is assumed to dissociate upon incidence so that the corresponding parameter value must be used for both B and F.

Remarks on implantation into a predamaged material

In the case of multiple implantations, the predamage caused by preceding implants influences the (de-)channeling behavior of the subsequently implanted ions (see e.g. Ref. 22). In the input dialog, the user is asked whether a predamage is to be considered. If yes, the name of the file containing the damage probability histogram of the previous implantation generated by the prof1z.exe analysis program (see below) must be given. The number and width of the depth intervals in the simulation of the preceding and the subsequent implantation must be identical. Of course it is also possible to generate a file with the (pre-)damage probability "by hand".

1.3 Choice of the width of depth intervals

In Crystal-TRIM simulations, a histogram representation is used for the range profile of the implanted ions and the other depth distributions. If the implanted projectiles come to rest, they are collected in certain depth intervals of the histogram. The maximum number of depth intervals is 400. The actual number of intervals and their width depends on the expected depth profile and the desired statistical accuracy of the histogram (narrow widths require longer simulations in order to avoid strongly fluctuating ordinate values). With some preliminary knowledge about the depth profile (e.g. SRIM simulations or experimental data) to be simulated, the width of the depth intervals can be chosen in the input dialog. Using the chosen width, the input dialog program estimates below which energy the projectile cannot leave a depth interval. The user can choose this energy or use another. In Crystal-TRIM the projectile motion is followed until this energy, then it is assumed to be at rest. This procedure is set up to save computing time. If the chosen histogram representation does not fit well, the user should repeat the simulation (with another choice in the input dialog).

1.4 Splitting procedure²⁾

This procedure may lead to a considerable increase of computational efficiency in cases where long channeling tails are expected. The ratio between the CPU-time of a simulation without splitting and the time of a calculation using this method may be about 5 to 10, if the same statistical accuracy is required for results of both simulations. The parameter used in the splitting procedure is ***SIGDEPTH***. This number describes how many projectiles contribute independently to the range (or depth) profile in a certain depth SIGDEPTH. The value of ***SIGDEPTH*** (usually between 5 and 20, but also dependent on the application) must be defined by the user during the input dialog. SIGDEPTH is determined at the end of simulations and is given in the output file ***name.OUT*** file (see below). The value of SIGDEPTH is important in order to estimate the statistical significance of long channeling tails of the simulated depth profiles: For depths > SIGDEPTH the range profile is due to <***SIGDEPTH*** projectile histories.

2. How to use Crystal-TRIM?

Step 1: Input dialog using the program xtru04.exe

command: **xtru04.exe**

All input parameters are asked for during the dialog. The dialog program creates the input files **name.IN** and **name.DAT**. **name** must exactly contain 4 ASCII characters. The dialog program also generates the names of the output files filled with data in *Step 2*.

Step 2: Crystal-TRIM simulation using the program xtr041.exe

command: **xtr041.exe < name.IN**

During the simulation, some informations on the status of the calculation are shown on the screen.

Description of the output files

name.OUT	file with a "listing" of input data and results, e.g. tables containing histograms of range and damage depth distributions, data on mean projected range and other depth profile parameters, and e.g. SIGDEPTH.
name.1Dn	file with a table of all depth profiles generated by the atomic component n of the (possibly) molecular ion ($1 \leq n \leq 3$), $n=1$ for atomic ions.
name.ST	is generated, but not relevant.

Step 3: Postprocessing using prof1z.exe

command: **prof1z.exe**

Using the input **name.1Dn**, this program generates different depth profiles for further graphical representation (e.g. by ORIGIN®). These files contain two-column tables where the depth (in nm) is the first one.

iopt=1	second column: depth profile of implanted ions in cm^{-3} . <i>Note: Since in many cases a logarithmic ordinate scale is used, in prof1z.exe the value "0" is replaced by the minimum, non-zero ordinate value. This might lead to some confusion if results show poor statistics.</i>
iopt=2	second column: nuclear energy deposition in $\text{eV}\times\text{cm}^{-3}$
iopt=3	second column: electronic energy deposition in $\text{eV}\times\text{cm}^{-3}$
iopt=4	second column: damage concentration in cm^{-3} (only valid in the single-crystalline substrate)

	<i>This is the concentration of the displaced atoms.</i>
iopt=5	second column: damage probability (only valid in the single-crystalline substrate) <i>These data may be used as input for simulation of ion implantation in the case of preexisting damage (see above).</i>

Note that options 4 and 5 are only relevant for simulations in which the damage accumulation is considered. Damage concentration equal to the atomic density of the substrate or damage probability equal 1 corresponds to amorphization. In this manner, the thickness of the amorphous layer formed during ion implantation can be determined.

1)References

Selected papers on Crystal-TRIM:

- [1] M. Posselt, J.P. Biersack: Computer simulation of ion implantation into crystalline targets, Nuclear Instruments and Methods B **64** (1992) 706.
- [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.
- [3] M. Posselt: Computer simulation of channeling implantation at high and medium energies, Nuclear Instruments and Methods B **80/81** (1993) 28.
- [4] M. Posselt: Computer simulation of channeling effects in ion implantation, Materials Research Society Symp. Proc. **279** (1993) 23.
- [5] C.S. Murthy, M. Posselt: Comparative study of simulated damage accumulation in silicon crystals, Electrochemical Society Proc. **93-6** (1993) 545.
- [6] M. Posselt: Channeling effects and defect accumulation in ion implantation, Nuclear Instruments and Methods B **90** (1994) 373.
- [7] M. Posselt: 3D modeling of ion implantation into crystalline silicon: influence of damage accumulation on dopant profiles, Nuclear Instruments and Methods B **96** (1995) 163.
- [8] M. Posselt: Dynamic simulation of damage accumulation during implantation of BF₂ molecular ions into crystalline silicon, Nuclear Instruments and Methods B **102** (1995) 167.
- [9] M. Posselt: Dynamic simulation of ultra-shallow implantation profiles in single crystalline silicon, Materials Research Society Symp. Proc. **389** (1995) 227.
- [10] C.S. Murthy, M. Posselt, T. Frei: Three-dimensional modeling of low-dose BF₂ implantation into single-crystalline silicon, J. Vac. Sc. & Technol. B **14** (1996) 278.
- [11] M. Posselt, B. Schmidt, C.S. Murthy, T. Feudel, and K. Suzuki: Modeling of damage accumulation during ion implantation into single-crystalline silicon, J. Electrochem. Soc. **144** (1997) 1495.
- [12] B. Schmidt, M. Posselt, N. Strecker, and T. Feudel: Atomistic simulation of ion implantation into 2d structures, Computational Materials Science **11** (1998) 87.
- [13] B. Schmidt, M. Posselt, N. Strecker, and T. Feudel: Atomistic modeling of ion implantation within a 2D process simulator, MRS Symp. Proc. **490** (1998) 21.
- [14] C.S. Murthy, M. Posselt, and T. Feudel: Physically-based modeling of two dimensional and three-dimensional implantation profiles: influence of damage accumulation, J. Vac. Sci. Technol. B **16** (1998) 440.
- [15] M. Posselt: Computer simulation of channeling profile analysis of implantation damage, MRS Symp. Proc. **532** (1998) 133.

- [16] W. Pilz, J. von Borany, R. Grötzschel, W. Jiang, M. Posselt, and B. Schmidt: Dependence of the silicon detector response to heavy ions on the direction of incidence: computer simulations versus experimental data, *Nucl. Instr. Meth. A* **419** (1998) 137.
- [17] T. Feudel, N. Strecker, U. Krause, B. Schmidt, and M. Posselt: Monte Carlo ion implantation simulation for deep ULSI transistors, *Proc. of the 1999 Semiconductor TCAD Workshop vol. 2*, p. 7.1, Hsinchu, May 1999.
- [18] M. Posselt, B. Schmidt, T. Feudel, N. Strecker: Atomistic simulation of ion implantation and its application in Si technology, *Materials Science and Engineering B* **71** (2000) 128.
- [19] M. Posselt, L. Bischoff, J. Teichert: Influence of dose rate and temperature on ion beam-induced defect evolution in Si investigated by channeling implantation at different doses, *Appl. Phys. Lett.* **79** (2001) 1444.
- [20] M. Posselt, L. Bischoff, J. Teichert, A. Ster: Influence of dynamic annealing on the shape of channeling implantation profiles in Si and SiC, *J. Appl. Phys.* **93** (2003) 1004.
- [21] M. Posselt, M. Mäder, R. Grötzschel, M. Behar: Competing influence of damage buildup and lattice vibrations on the shape of ion range profiles in Si, *Appl. Phys. Lett.* **83** (2003) 545.
- [22] M. Posselt, M. Mäder, A. Lebedev, R. Grötzschel: Multiple implantations into Si: influence of the implantation sequence on ion range profiles, *Appl. Phys. Lett.* **87** (2005) 043109.
- [23] M. Posselt, L. Bischoff, D. Grambole, F. Herrmann: Competition between damage buildup and dynamic annealing in ion implantation into Ge, *Appl. Phys. Lett.* **89** (2006) 151918.
- [24] M. Radek, H. Bracht, M. Posselt, B. Liedke, B. Schmidt, D. Bougeard: Temperature dependence of ion-beam mixing in crystalline and amorphous germanium isotope multilayer structures, *J. Appl. Phys.* **115** (2014) 023506.
- [25] A. M. Jakob, S. G. Robson, V. Schmitt, V. Mourik, M. Posselt, D. Spemann, B. C. Johnson, H. R. Firgau, E. Mayes, J. C. McCallum, A. Morello, D. N. Jamieson: Deterministic Shallow Dopant implantation in silicon with detection confidence upper-bound to 99.85% by ion–solid interactions, *Adv. Mater* **34** (2022) 2103235.

2) Acknowledgements

The data file scoef1.dat corresponds to the data file scoef.dat published in Ref. [a]. The data file scoef2.dat corresponds to the corrected scoef.dat file used in 1989 and later in the standard TRIM code [a, b]. In the above references¹⁾ the file scoef1.dat was always 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 material 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. Hagmark, *Nuclear Instruments and Methods* **174** (1980) 257.

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