

Standard Crystal-TRIM

Manual 2025

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History

The Crystal-TRIM code has been developed by Matthias Posselt (Helmholtz-Zentrum Dresden – Rossendorf[§], Institute of Ion Beam Physics and Materials Research) since 1991. The main program development took place during the nineties of the last century. Parts of the package are based on the TRIM (Transport of Ions in Matter) program of Biersack et al. [a,b], published in Ref. [a]. TRIM was designed to simulate ion implantation into amorphous solids. Now TRIM it is part of the SRIM package of Ziegler, which can be downloaded from <http://www.srim.org/>. In contrast the purpose of Crystal-TRIM is the simulation of ion implantation into single-crystalline solids, details are given below. The present version of Crystal-TRIM (also called Standard Crystal-TRIM) is the result of the last comprehensive revision in May 2004. Main publications with Crystal-TRIM results are given in the reference list below.

Besides the Standard Crystal-TRIM various other special codes exist, e.g. as part of the (semiconductor technology) 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/were part of the TCAD software of Synopsys®.

Range of application, models and parameters

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, as synonym, high fluence) implantation cannot be described. Note, that the values of the semiempirical parameters for electronic stopping and damage accumulation given below are only valid for the case with a single-crystalline Si (c-Si) substrate. These data were obtained by comparison of simulation results with experimental (SIMS) depth profiles.

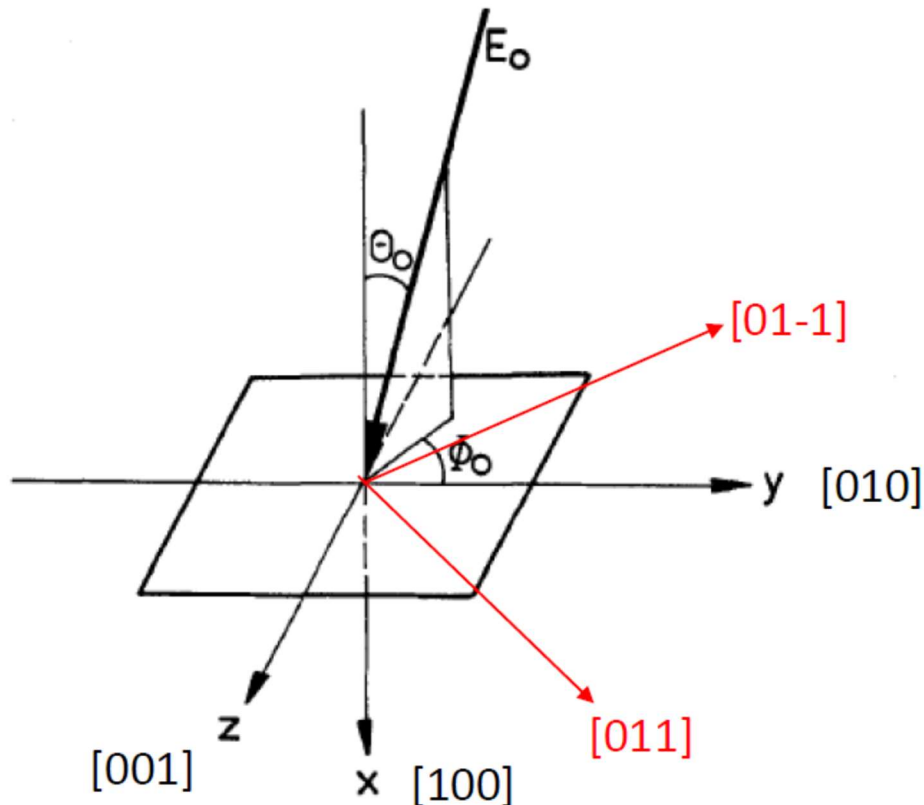
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The physical background of Crystal-TRIM is described in the papers given in the reference list below. Main applications of the code were investigations on channeling effects and the influence of damage accumulation during ion bombardment on channeling. Like TRIM, Crystal-TRIM uses the binary collision approximation to treat the collisions between the incident ion with target atoms. The trajectories of these projectiles are followed until they come to rest. During their slowing down these energetic particles generate so-called primary knock-on atoms which may initiate collision cascades. These cascades are not simulated explicitly, but the corresponding nuclear and electronic energy deposition is registered.

The present version can be used to calculate as-implanted range and damage distributions as a function of depth. An efficient splitting procedure may 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 (visible on a logarithmic concentration scale) are of interest since these determine the depth of the p-n junction (in the case of implantation of p- or n-dopants).

Note that in Crystal-TRIM the ion energy (E_0) is always the kinetic energy of the ion. In most practically relevant cases of ion implantation the ions are quickly neutralized after impact so that the ion charge is not considered in the code. The number of ion (or projectile) histories used in the simulation must be less than 10^9 . It should be noticed that, in case of considering damage accumulation, each projectile represents a certain ion dose (or fluence). In the following, the terms “ion” and “projectile” are used as synonyms, and this may be also a molecular ion or projectile.

The following geometry is implemented in Crystal-TRIM: The tilt angle θ_0 is defined with respect to the surface normal. The figure shows the case of a (100) substrate where the surface normal is (anti)parallel to the [100] direction. The rotation or twist angle Φ_0 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, which must be used in Crystal-TRIM.



Semi-empirical parameters used in the code

In Crystal-TRIM, few semi-empirical parameters are used. Apart from their default values already implemented, special values can be used which were/can be obtained by comparing simulation results with experimental depth profiles in c-Si, which are preferentially measured by SIMS.

Parameters of the electronic stopping models

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

clambda: Determines the “random peak” of the ion range (depth) profile, i.e. is not directly related to channeling. The position of this peak would be almost the same if the material were amorphous. The default value of clambda is around 1 and is provided by the (*using xtru04.exe*) *scoef*.dat* file. 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 deeper channeling parts of the range profiles. 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 the projectile on the distance to the nearest target atom.

In order to obtain the values of clambda and Cel from experimental SIMS depth profiles, use the following approach: (i) Consider a depth profile for implantation into a non-channeling direction (best: 7° tilt, 22.5° rotation) and fit clambda to get the same peak position. (ii) Consider a depth profile for implantation into the [100] channeling direction (0° tilt) and fit Cel to the profile shape (especially the deeper channeling part). Note that also the thickness of the amorphous surface layer and other factors may influence the shape of channeling implantation profiles.

Recommended values of Cel (and Cel110) in special cases:

The following numbers are examples used in previous studies on ion implantation into c-Si.

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

Note that the BF₂ projectile is assumed to dissociate upon incidence, therefore use the corresponding values for B *and* F.

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

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 increased dechanneling of the subsequently implanted ions. 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 list 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 (amorphous 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 around the tetrahedral site, 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*cacc)% of the total damage remains before the next projectile impact, in general **cacc** ≤ 1 should be used

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*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*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*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*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***ccrit**)%

The following table shows recommended values of the parameters **cacc** and **ccrit** for typical examples (for model 6)

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 (**xtru04.exe**), 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 preceding implantation generated by the prof1z.exe postprocessing program 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”.

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, e.g. for nuclear and electronic energy deposition. 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 **xtru04.exe**. 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 a smaller. In Crystal-TRIM the projectile motion is followed until this energy, then the projectile 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 of the interval width in the input dialog **xtru04.exe**).

Splitting procedure [c]

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*** (should be usually between 5 and 20, but also depends on the application) must be defined by the user during the input dialog **xtru04.exe** if the “splitting option” is chosen. **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.

How to use Crystal-TRIM?

Step 1: Input dialog using the program xtru04.exe

command: **xtru04.exe** (or ./xtru04.exe on a Linux system)

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. Do not change the file **name.DAT**! The dialog program also generates the names of the Crystal-TRIM output files. Also, in this code many parameters for the **name.DAT** file are defined (default values) and need not be given by the user.

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

command: **xtr041.exe < name.IN** (or ./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. number of backscattered projectiles and 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** (or with ./prof1z.exe)

Using the input **name.1Dn**, this program generates different depth profiles for further graphical representation (e.g. by Origin Lab®). 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 $\text{eV} \times \text{cm}^{-3}$

<i>iopt=4</i>	second column: damage concentration in cm ⁻³ (only valid in the single-crystalline substrate) <i>This is the concentration of the displaced atoms.</i>
<i>iopt=5</i>	second column: damage probability (only valid in the single-crystalline substrate if a damage accumulation model is considered) <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.

The postprocessing program asks for the backscattering yield. This number can be obtained by dividing the number of backscattered projectiles (particles) given in the *OUT file by the total number of projectile histories simulated. In most cases, the backscattering yield is small so that one can also choose zero.

Note that using **prof1zmuem.exe**, in the first column of the output file the depth is given in micrometer.

Crystal-TRIM for Linux and Windows

The Standard Crystal-TRIM package consists of the following Fortran source codes:

Dialog to create the necessary input files: **xtru04.f**

Main part (simulation of ion implantation): **xtr041.f**

Postprocessing to create output files suitable for graphical representation (e.g. using Origin Lab®) : **prof1z.f** (or **prof1zmuem.f**, see above).

Note, that the code was developed step by step for different applications which is reflected by the complex and somewhat unclear structure of the Fortran sources. The Standard Crystal-TRIM is only one of these applications so that there are some source files and parts of source files that are not relevant here.

*The different routines and the most relevant parameters are described in the source files on lines marked by **c 25-**. Other comment lines in the source files are not relevant. In particular, in the subroutine PRO981 (of xtr041.f) the treatment of the motion of the projectiles in the target is described.*

Generation of executables from Fortran sources

Compilation under **Linux** on command line:

ifort -static -r8 -O3 -o name_of_executable.exe name_of_source.f

where ifort is the installed Intel® Fortran compiler. Ignore the warnings appearing during the compilation.

Compilation under **Windows** on Intel® oneAPI command prompt for Intel® 64 for Visual Studio:

```
ifx -static -xR8 -O3 -o name_of_executable.exe name_of_source.f
```

where ifx is the installed Intel® Fortran compiler. Ignore the warnings appearing during the compilation.

The following data files and executables are necessary for all applications of Crystal-TRIM:

scoef1.dat, scoef2.dat, xtru04.exe, xtr041.exe, prof1z.exe (or prof1zmuem.exe)

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 code ([a] and <http://www.srim.org/>). In most of the previous Crystal-TRIM calculations (see reference list below) the file scoef1.dat was used.

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. It should be also noted that under MSDOS the executables should be run on a local PC drive (instead of a network drive). This can avoid problems with paths and environments.

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