Standard Crystal-TRIM

Tutorials 2025

The following shows some applications of the code with inputs and outputs appearing on the computer monitor.
The commands (on the command line) and the data to be given by the user are shown in bold face. The commands are in the style for the MSDOS version. If the linux version is used the commands must begin with **./**
In the following examples the computing time is mostly less than 10 minutes (valid for calculations on both linux and MSDOS systems). The input and output data files can be found in the corresponding folders.
The diagrams shown below were generated using Origin Lab®.

Example A:
100 keV B into (100) Si, 10^{14} cm^{-2}, 0° tilt, 0° rotation
15 Å SiO_2 amorphous top layer

Calculation without considering damage accumulation since this effect is not relevant here.

Step 1: Input dialog using the program xtru04.exe

xtru04.exe

Crystal-TRIM
developed by Matthias Posselt
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Input Dialog

File names consist of a variable first part
and a constant second part.
Name of the first part?(exactly 4 ASCII characters!)
b1ha
substrate:
single-crystalline Si (1)?

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single-crystalline Ge (2)?
diamond (3)?
1
Ion
Energy in keV?
100
Orientation of the substrate surface (e.g. 1 0 0) ?

Insert a space between the integers!
Please note: Only (100),(110) and (111) surfaces can
be considered!
1 0 0
Tilt angle theta0 in deg.?
0
Rotation angle phi0 in deg.)?
0
Name of the file which contains the parameters
for ZBL electronic stopping?
scoef1.dat - original ZBL 1985 (1)
scoef2.dat - 1989 (2)
scoef1.dat = default in previous Crystal-TRIM applications
1
Atomic (1) or molecular (2) ion?
1
Atomic number?
5
Mass: most abundant isotope (1), another (2)
1
clambda is 1.010

use this standard value (yes 1, no 2)?
1
Cel and Cel110 different from 1? (no 1, yes 2)
1
Number of ion histories to be simulated?
10000
Use of an efficient splitting procedure
to improve the statistical precision (no 1, yes 2)?
Splitting is particularly recommended in cases
where long channeling tails are expected.
1
Number of amorphous layers on top of
the single-crystalline substrate (Max.:10):
1
Layer 1 --Thickness (Angstrom)?
(total thickness of layers must not exceed 1e+05 A)
15
Density (g/cm-3)?
2.24
SiO2 (1) or another layer (2)?
1
Crystalline substrate:
Temperature different from RT (300K)? (no 1, yes 2)
1
Consideration of damage accumulation
(phenomenological models)? (no 1, yes 2)

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```
1
  Width of the intervals in the histograms (A)?
  Maximum number of depth intervals is 400
100
  Final energy in the simulation of
  the motion of the ions?
   Estimation:
    E(keV)        Range(A)
    0.500E+00     0.273E+02
   Final energy in the simulation of
   the motion of the ions (keV)?
0.5
       writing to input file     b1ha.DAT
```

The input data files b1ha.IN and b1ha.DAT have been written.

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

xtr041.exe < b1ha.IN

```
       start in981
       reading from input file     b1ha.DAT
       input file closed
       end in981
       start sec971
       end sec971
       start pro981
 status of calculation in %    particle histories
          10                  1000
          20                  1999
          30                  2998
          40                  3997
          50                  4996
          60                  5995
          70                  6994
          80                  7993
          90                  8992
         100                   9991
       end pro981
       start out981
       writing to output file     b1ha.OUT
       writing to output file     b1ha.1D1
       output file   b1ha.1D1        closed
       output file   b1ha.OUT        closed
       end out981
```

The output data files b1ha.OUT, b1ha.1D1 and b1ha.ST have been written. Only b1ha.1D1 is relevant for following postprocessing.

Step 3: Postprocessing using prof1z.exe

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prof1z.exe

program prof1z
input data file?
(not more than 12 ASCII characters)

b1ha.1D1

output data file?
(not more than 14 ASCII characters)

b1harange.dat

options:
iopt
1 range profile
2 nuclear energy deposition
3 electronic energy deposition
4 damage concentration (only valid in c-Si)
5 damage probability (only valid in c-Si)

iopt?

1

backscattering yield (see file "name.OUT")?

0.

dose (cm**(-2)?

1.e14

reading from input file b1ha.1D1
input file b1ha.1D1 closed
writing to output file b1harange.dat
output file b1harange.dat closed

Example B:

100 keV B into (100) Si, 10^{14} cm^{-2}, 7° tilt, 22.5° rotation 15 Å SiO_2 amorphous top layer

Calculation without considering damage accumulation since this effect is not relevant here.

Step 1: Input dialog using the program xtru04.exe

xtru04.exe

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Input Dialog

File names consist of a variable first part

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and a constant second part.
Name of the first part?(exactly 4 ASCII characters!)
b1hb
substrate:
single-crystalline Si (1)?
single-crystalline Ge (2)?
diamond (3)?
1
Ion
Energy in keV?
100
Orientation of the substrate surface (e.g. 1 0 0) ?

Insert a space between the integers!
Please note: Only (100),(110) and (111) surfaces can
be considered!
1 0 0
Tilt angle theta0 in deg.?
7
Rotation angle phi0 in deg.)?
22.5
Name of the file which contains the parameters
for ZBL electronic stopping?
scoef1.dat - original ZBL 1985 (1)
scoef2.dat - 1989 (2)
scoef1.dat = default in previous Crystal-TRIM applications
1
Atomic (1) or molecular (2) ion?
1
Atomic number?
5
Mass: most abundant isotope (1), another (2)
1
clambda is 1.010

use this standard value (yes 1, no 2)?
1
Cel and Cel110 different from 1? (no 1, yes 2)
1
Number of ion histories to be simulated?
10000
Use of an efficient splitting procedure
to improve the statistical precision (no 1, yes 2)?
Splitting is particularly recommended in cases
where long channeling tails are expected.
2
Measure of the statistical precision of simulation
results: ISIGDEPTH?
20
Number of amorphous layers on top of
the single-crystalline substrate (Max.:10):
1
Layer 1 --Thickness (Angstrom)?
(total thickness of layers must not exceed 1e+05 A)
15
Density (g/cm-3)?

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2.24
SiO2 (1) or another layer (2)?
1
Crystalline substrate:
Temperature different from RT (300K)? (no 1, yes 2)
1
Consideration of damage accumulation
(phenomenological models)? (no 1, yes 2)
1
Width of the intervals in the histograms (A)?
Maximum number of depth intervals is 400
100
Final energy in the simulation of
the motion of the ions?
Estimation:
E(keV) Range(A)
0.500E+00 0.273E+02
Final energy in the simulation of
the motion of the ions (keV)?
0.5
writing to input file b1hb.DAT

The input data files b1hb.IN and b1hb.DAT have been written.

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

xtr041.exe < b1hb.IN

```
start in981
reading from input file     b1hb.DAT
input file closed
end in981
start sec971
end sec971
start pro981
status of calculation in %    particle histories
  10                  1000
  20                  1999
  30                  2998
  40                  3997
  50                  4996
  60                  5995
  70                  6994
  80                  7993
  90                  8992
 100                  9991
end pro981
start out981
writing to output file     b1hb.OUT
writing to output file     b1hb.1D1
output file   b1hb.1D1        closed
output file   b1hb.OUT        closed
end out981
```


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The output data files b1hb.OUT, b1hb.1D1 and b1hb.ST have been written. Only b1hb.1D1 is relevant for following postprocessing.

Step 3: Postprocessing using prof1z.exe

prof1z.exe

program prof1z
input data file?
(not more than 12 ASCII characters)

b1hb.1D1

output data file?
(not more than 14 ASCII characters)

b1hbrange.dat

options:
iopt
1 range profile
2 nuclear energy deposition
3 electronic energy deposition
4 damage concentration (only valid in c-Si)
5 damage probability (only valid in c-Si)

iopt?

1

backscattering yield (see file "name.OUT")?

0.

dose (cm**(-2)?

1.e14

reading from input file b1hb.1D1
input file b1hb.1D1 closed
writing to output file b1hbrange.dat
output file b1hbrange.dat closed

<u>Graphical representation of B depth profiles for Examples A and B</u>

The following diagrams show the B depth profiles b1harange.dat and b1hbrange.dat. Note the logarithmic scale on the ordinate, which is relevant for implantation of electrical dopants in order to determine the location of the p-n junction. The logarithmic scale shows the so-called channeling tail in the case of 7° tilt implantation. If the Si substrate were amorphous this tail would not exist and after the peak the decrease would be very steep.

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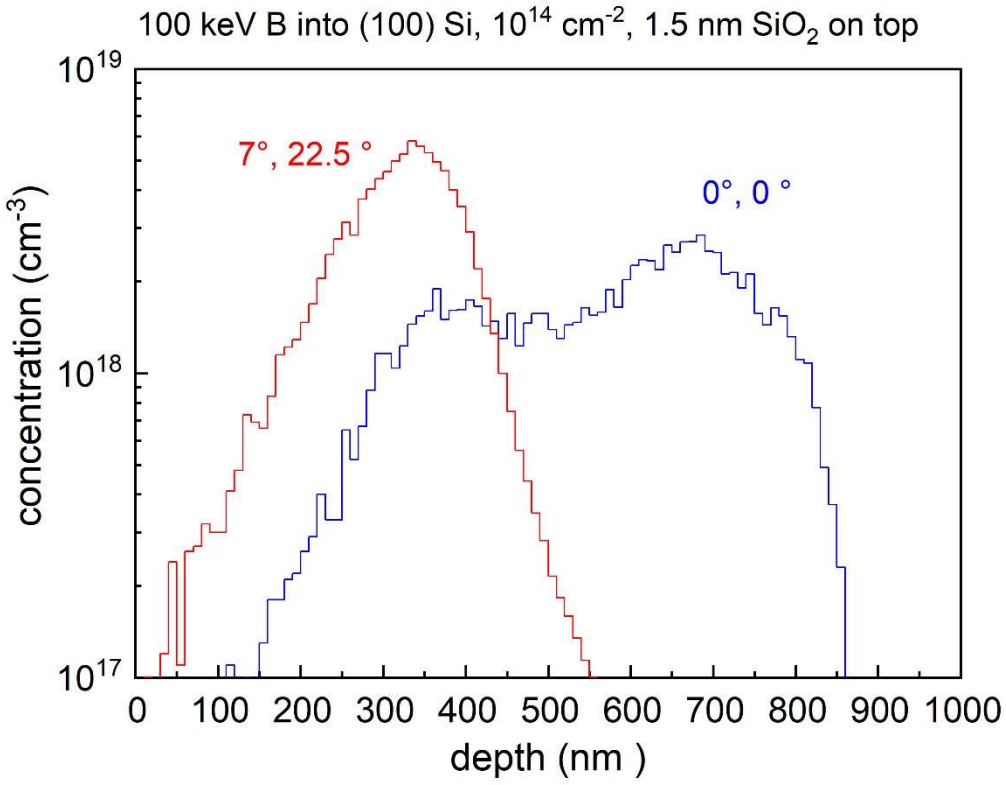

The data shown were calculated using MSDOS executables on a certain Windows system. On various systems and processors, the individual numbers may be not identical. However, all these results are statistically not different. This holds for calculations under MSDOS and Linux.

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Example C
100 keV P into (100) Si, 10^{15} cm^{-2}, 0° tilt, 0° rotation
15 Å SiO_2 amorphous top layer

Calculation without considering damage accumulation.

Step 1: Input dialog using the program xtru04.exe

xtru04.exe

```
        Crystal-TRIM
         developed by Matthias Posselt
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         Helmholtz-Zentrum Dresden-Rossendorf
         Institute of Ion Beam Physics and
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         D-01328 Dresden, Germany


         Input Dialog


   File names consist of a variable first part
   and a constant second part.
   Name of the first part?(exactly 4 ASCII characters!)
p1ha
   substrate:
   single-crystalline Si (1)?
   single-crystalline Ge (2)?
   diamond (3)?
1
   Ion
     Energy in keV?
100
     Orientation of the substrate surface (e.g. 1 0 0) ?

Insert a space between the integers!
     Please note: Only (100),(110) and (111) surfaces can
     be considered!
1 0 0
     Tilt angle theta0 in deg.?
0
     Rotation angle phi0 in deg.)?
0
     Name of the file which contains the parameters
     for ZBL electronic stopping?
     scoef1.dat - original ZBL 1985 (1)
     scoef2.dat - 1989 (2)
     scoef1.dat = default in previous Crystal-TRIM applications
1
```


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Atomic (1) or molecular (2) ion?
1
Atomic number?
15
Mass: most abundant isotope (1), another (2)
1
clambda is 1.000

use this standard value (yes 1, no 2)?
1
Cel and Cel110 different from 1? (no 1, yes 2)
2
Cel110?
0.97
Cel?
1.45
Number of ion histories to be simulated?
10000
Use of an efficient splitting procedure
to improve the statistical precision (no 1, yes 2)?
Splitting is particularly recommended in cases
where long channeling tails are expected.
1
Number of amorphous layers on top of
the single-crystalline substrate (Max.:10):
1
Layer 1 --Thickness (Angstrom)?
(total thickness of layers must not exceed 1e+05 A)
15
Density (g/cm-3)?
2.24
SiO2 (1) or another layer (2)?
1
Crystalline substrate:
Temperature different from RT (300K)? (no 1, yes 2)
1
Consideration of damage accumulation
(phenomenological models)? (no 1, yes 2)
1
Width of the intervals in the histograms (A)?
Maximum number of depth intervals is 400
50
Final energy in the simulation of
the motion of the ions?
Estimation:
E(keV) Range(A)
0.300E+00 0.127E+02
Final energy in the simulation of
the motion of the ions (keV)?
0.3
writing to input file p1ha.DAT

The input data files p1ha.IN and p1ha.DAT have been written.

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

xtr041.exe < p1ha.IN

```
        start in981
        reading from input file     p1ha.DAT
        input file closed
        end in981
        start sec971
        end sec971
        start pro981
 status of calculation in %    particle histories
           10                  1000
           20                  1999
           30                  2998
           40                  3997
           50                  4996
           60                  5995
           70                  6994
           80                  7993
           90                  8992
          100                   9991
        end pro981
        start out981
        writing to output file     p1ha.OUT
        writing to output file     p1ha.1D1
        output file   p1ha.1D1         closed
        output file   p1ha.OUT         closed
        end out981
```

The output data files p1ha.OUT, p1ha.1D1 and p1ha.ST have been written. Only p1ha.1D1 is relevant for following postprocessing.

Step 3: Postprocessing using prof1z.exe

prof1z.exe

```
            program prof1z
            input data file?
            (not more than 12 ASCII characters)
```

p1ha.1D1

```
            output data file?
            (not more than 14 ASCII characters)
```

p1harange.dat

```
              options:
              iopt
              1       range profile
              2       nuclear energy deposition
              3       electronic energy deposition
              4       damage concentration (only valid in c-Si)
              5       damage probability (only valid in c-Si)         iopt?
```

1

```
      backscattering yield (see file "name.OUT")?
```


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0.

dose (cm**(-2)?

1.e15

reading from input file p1ha.1D1
input file p1ha.1D1 closed
writing to output file p1harange.dat
output file p1harange.dat closed

Example D

100 keV P into (100) Si, 10^{15} cm^{-2}, 7° tilt, 22.5° rotation 15 Å SiO_2 amorphous top layer

Calculation without considering damage accumulation.

Step 1: Input dialog using the program xtru04.exe

xtru04.exe

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Input Dialog

File names consist of a variable first part
and a constant second part.
Name of the first part?(exactly 4 ASCII characters!)

p1hb

substrate:
single-crystalline Si (1)?
single-crystalline Ge (2)?
diamond (3)?

1

Ion
Energy in keV?

100

Orientation of the substrate surface (e.g. 1 0 0) ?

Insert a space between the integers!
Please note: Only (100),(110) and (111) surfaces can
be considered!

1 0 0

Tilt angle theta0 in deg.?

7

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Rotation angle phi0 in deg.)?
22.5
Name of the file which contains the parameters
for ZBL electronic stopping?
scoef1.dat - original ZBL 1985 (1)
scoef2.dat - 1989 (2)
scoef1.dat = default in previous Crystal-TRIM applications
1
Atomic (1) or molecular (2) ion?
1
Atomic number?
15
Mass: most abundant isotope (1), another (2)
1
clambda is 1.000

use this standard value (yes 1, no 2)?
1
Cel and Cel110 different from 1? (no 1, yes 2)
2
Cel110?
0.97
Cel?
1.45
Number of ion histories to be simulated?
10000
Use of an efficient splitting procedure
to improve the statistical precision (no 1, yes 2)?
Splitting is particularly recommended in cases
where long channeling tails are expected.
2
Measure of the statistical precision of simulation
results: ISIGDEPTH?
20
Number of amorphous layers on top of
the single-crystalline substrate (Max.:10):
1
Layer 1 --Thickness (Angstrom)?
(total thickness of layers must not exceed 1e+05 A)
15
Density (g/cm-3)?
2.24
SiO2 (1) or another layer (2)?
1
Crystalline substrate:
Temperature different from RT (300K)? (no 1, yes 2)
1
Consideration of damage accumulation
(phenomenological models)? (no 1, yes 2)
1
Width of the intervals in the histograms (A)?
Maximum number of depth intervals is 400
50
Final energy in the simulation of
the motion of the ions?
Estimation:

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```
 E(keV)        Range(A)
 0.300E+00     0.127E+02
Final energy in the simulation of
the motion of the ions (keV)?
```
0.3
```
      writing to input file     p1hb.DAT
```

The input data files p1hb.IN and p1hb.DAT have been written.

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

xtr041.exe < p1hb.IN

```
      start in981
      reading from input file     p1hb.DAT
      input file closed
      end in981
      start sec971
      end sec971
      start pro981
 status of calculation in %    particle histories
        10                  1000
        20                  1999
        30                  2998
        40                  3997
        50                  4996
        60                  5995
        70                  6994
        80                  7993
        90                  8992
       100                   9991
      end pro981
      start out981
      writing to output file     p1hb.OUT
      writing to output file     p1hb.1D1
      output file   p1hb.1D1        closed
      output file   p1hb.OUT        closed
      end out981
```

The output data files p1hb.OUT, p1hb.1D1 and p1hb.ST have been written. Only p1hb.1D1 is relevant for following postprocessing.

Step 3: Postprocessing using prof1z.exe

prof1z.exe
```
            program prof1z
            input data file?
            (not more than 12 ASCII characters)
```
p1hb.1D1
```
            output data file?
            (not more than 14 ASCII characters)
```
p1hbrange.dat

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options:
iopt
1 range profile
2 nuclear energy deposition
3 electronic energy deposition
4 damage concentration (only valid in c-Si)
5 damage probability (only valid in c-Si) iopt?

1

backscattering yield (see file "name.OUT")?

0.

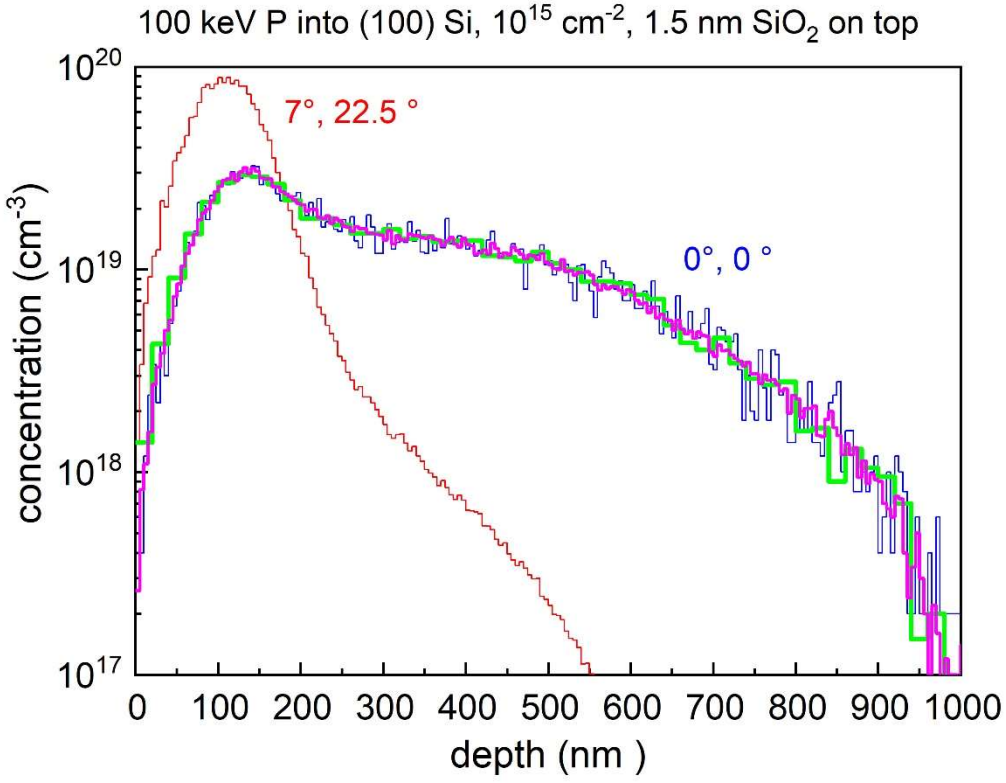
dose (cm**(-2)?

1.e15

reading from input file p1hb.1D1
input file p1hb.1D1 closed
writing to output file p1hbrange.dat
output file p1hbrange.dat closed

Graphical representation of P depth profiles for Examples C and D

The following diagram shows the P depth profiles p1harange.dat (blue) and p1hbrange.dat (red). Note that in the case of 0° implantation the interval width is too small to give a "good statistical shape" of the profile. Improvements: Either use a larger interval width or a more projectile (ion) histories (more that 10000). For comparison, the green histogram shows a depth profile for 0° implantation with an interval width of 200 Å instead of 50 Å. The magenta histogram shows results of simulation with 100000 projectile histories instead of 10000.



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Example E
100 keV P into (100) Si, 10^{15} cm^{-2}, 0° tilt, 0° rotation
15 Å SiO_2 amorphous top layer

Calculation with considering damage accumulation.

Step 1: Input dialog using the program xtru04.exe

xtru04.exe

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Input Dialog

File names consist of a variable first part
and a constant second part.
Name of the first part?(exactly 4 ASCII characters!)
p1hc
substrate:
single-crystalline Si (1)?
single-crystalline Ge (2)?
diamond (3)?
1
Ion
Energy in keV?
100
Orientation of the substrate surface (e.g. 1 0 0) ?

Insert a space between the integers!
Please note: Only (100),(110) and (111) surfaces can
be considered!
1 0 0
Tilt angle theta0 in deg.?
0
Rotation angle phi0 in deg.)?
0
Name of the file which contains the parameters
for ZBL electronic stopping?
scoef1.dat - original ZBL 1985 (1)
scoef2.dat - 1989 (2)
scoef1.dat = default in previous Crystal-TRIM applications
1

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Atomic (1) or molecular (2) ion?
1
Atomic number?
15
Mass: most abundant isotope (1), another (2)
1
clambda is 1.000

use this standard value (yes 1, no 2)?
1
Cel and Cel110 different from 1? (no 1, yes 2)
2
Cel110?
0.97
Cel?
1.45
Number of ion histories to be simulated?
10000
Use of an efficient splitting procedure
to improve the statistical precision (no 1, yes 2)?
Splitting is particularly recommended in cases
where long channeling tails are expected.
2
Measure of the statistical precision of simulation
results: ISIGDEPTH?
20
Number of amorphous layers on top of
the single-crystalline substrate (Max.:10):
1
Layer 1 --Thickness (Angstrom)?
(total thickness of layers must not exceed 1e+05 A)
15
Density (g/cm-3)?
2.24
SiO2 (1) or another layer (2)?
1
Crystalline substrate:
Temperature different from RT (300K)? (no 1, yes 2)
1
Consideration of damage accumulation
(phenomenological models)? (no 1, yes 2)
2
Model number (1,2,3,4,5,6)?
6
cacc? (between 0. and 1.)?
0.2
ccrit (between 0. and 1.)?
0.1
Dose (cm**(-2)) ?
1.e15
Does a predamage exist? (no 1, yes 2)
1
Width of the intervals in the histograms (A)?
Maximum number of depth intervals is 400
50
Final energy in the simulation of

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```
  the motion of the ions?
   Estimation:
    E(keV)        Range(A)
    0.300E+00     0.127E+02
   Final energy in the simulation of
   the motion of the ions (keV)?
0.3
       writing to input file     p1hc.DAT
```

The input data files p1hc.IN and p1hc.DAT have been written.

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

xtr041.exe < p1hc.IN

```
       start in981
       reading from input file     p1hc.DAT
       input file closed
       end in981
       start sec971
       end sec971
       start pro981
status of calculation in %    particle histories
         10                  1000
         20                  1999
         30                  2998
         40                  3997
         50                  4996
         60                  5995
         70                  6995
         80                  7993
         90                  8993
        100                  9991
       end pro981
       start out981
       writing to output file     p1hc.OUT
       writing to output file     p1hc.1D1
       output file   p1hc.1D1        closed
       output file   p1hc.OUT        closed
       end out981
```

The output data files p1hc.OUT, p1hc.1D1 and p1hc.ST have been written. Only p1hc.1D1 is relevant for following postprocessing.

Step 3: Postprocessing using prof1z.exe

prof1z.exe

```
       program prof1z
       input data file?
       (not more than 12 ASCII characters)
```


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p1hc.1D1

output data file?
(not more than 14 ASCII characters)

p1hcrange.dat

options:
iopt
1 range profile
2 nuclear energy deposition
3 electronic energy deposition
4 damage concentration (only valid in c-Si)
5 damage probability (only valid in c-Si)

iopt?

1

backscattering yield (see file "name.OUT")?

0.

dose (cm**(-2)?

1.e15

reading from input file p1hc.1D1
input file p1hc.1D1 closed
writing to output file p1hcrange.dat
output file p1hcrange.dat closed

Additionally: calculation of the damage (or amorphization) probability:

prof1z.exe

program prof1z
input data file?
(not more than 12 ASCII characters)

p1hc.1D1

output data file?
(not more than 14 ASCII characters)

p1hcopt5.dat

options:
iopt
1 range profile
2 nuclear energy deposition
3 electronic energy deposition
4 damage concentration (only valid in c-Si)
5 damage probability (only valid in c-Si)

iopt?

5

backscattering yield (see file "name.OUT")?

0.

atomic density of the single-crystalline substrate
in Angstroem**-3 (see ARHO in "name.OUT")?

0.05

dose (cm**(-2)?

1.e15

reading from input file p1hc.1D1
input file p1hc.1D1 closed
writing to output file p1hcopt5.dat
output file p1hopt5.dat closed

Note that the 0.05 is the *approximate* value of the atomic density of Si.

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Example F
100 keV P into (100) Si, 10^{15} cm^{-2}, 7° tilt, 22.5° rotation
15 Å SiO_2 amorphous top layer

Calculation with considering damage accumulation.

Step 1: Input dialog using the program xtru04.exe

xtru04.exe

```
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        developed by Matthias Posselt
        (C) Since 1991 by
        Matthias Posselt
        Helmholtz-Zentrum Dresden-Rossendorf
        Institute of Ion Beam Physics and
        Materials Research
        Bautzner Landstr. 400
        D-01328 Dresden, Germany


        Input Dialog


  File names consist of a variable first part
  and a constant second part.
  Name of the first part?(exactly 4 ASCII characters!)
p1hd
  substrate:
  single-crystalline Si (1)?
  single-crystalline Ge (2)?
  diamond (3)?
1
  Ion
    Energy in keV?
100
    Orientation of the substrate surface (e.g. 1 0 0) ?

Insert a space between the integers!
    Please note: Only (100),(110) and (111) surfaces can
    be considered!
1 0 0
    Tilt angle theta0 in deg.?
7
    Rotation angle phi0 in deg.)?
22.5
    Name of the file which contains the parameters
    for ZBL electronic stopping?
    scoef1.dat - original ZBL 1985 (1)
    scoef2.dat - 1989 (2)
    scoef1.dat = default in previous Crystal-TRIM applications
1
```


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Atomic (1) or molecular (2) ion?
1
Atomic number?
15
Mass: most abundant isotope (1), another (2)
1
clambda is 1.000

use this standard value (yes 1, no 2)?
1
Cel and Cel110 different from 1? (no 1, yes 2)
2
Cel110?
0.97
Cel?
1.45
Number of ion histories to be simulated?
10000
Use of an efficient splitting procedure
to improve the statistical precision (no 1, yes 2)?
Splitting is particularly recommended in cases
where long channeling tails are expected.
2
Measure of the statistical precision of simulation
results: ISIGDEPTH?
20
Number of amorphous layers on top of
the single-crystalline substrate (Max.:10):
1
Layer 1 --Thickness (Angstrom)?
(total thickness of layers must not exceed 1e+05 A)
15
Density (g/cm-3)?
2.24
SiO2 (1) or another layer (2)?
1
Crystalline substrate:
Temperature different from RT (300K)? (no 1, yes 2)
1
Consideration of damage accumulation
(phenomenological models)? (no 1, yes 2)
2
Model number (1,2,3,4,5,6)?
6
cacc? (between 0. and 1.)?
0.2
ccrit (between 0. and 1.)?
0.1
Dose (cm**(-2)) ?
1.e15
Does a predamage exist? (no 1, yes 2)
1
Width of the intervals in the histograms (A)?
Maximum number of depth intervals is 400
50
Final energy in the simulation of

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```
  the motion of the ions?
   Estimation:
    E(keV)        Range(A)
    0.300E+00     0.127E+02
   Final energy in the simulation of
   the motion of the ions (keV)?
```
0.3
```
       writing to input file     p1hd.DAT
```

The input data files p1hd.IN and p1hd.DAT have been written.

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

xtr041.exe < p1hd.IN

```
       start in981
        reading from input file     p1hd.DAT
        input file closed
        end in981
        start sec971
        end sec971
        start pro981
 status of calculation in %    particle histories
           10                  1000
           20                  1999
           30                  2998
           40                  3997
           50                  4996
           60                  5995
           70                  6994
           80                  7994
           90                  8992
          100                   9992
        end pro981
        start out981
        writing to output file     p1hd.OUT
        writing to output file     p1hd.1D1
        output file   p1hd.1D1        closed
        output file   p1hd.OUT        closed
        end out981
```

The output data files p1hd.OUT, p1hd.1D1 and p1hd.ST have been written. Only p1hd.1D1 is relevant for following postprocessing.

Step 3: Postprocessing using prof1z.exe

prof1z.exe

```
              program prof1z
              input data file?
              (not more than 12 ASCII characters)
```
p1hd.1D1

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output data file?
(not more than 14 ASCII characters)
p1hdrange.dat
options:
iopt
1 range profile
2 nuclear energy deposition
3 electronic energy deposition
4 damage concentration (only valid in c-Si)
5 damage probability (only valid in c-Si)
iopt?
1
backscattering yield (see file "name.OUT")?
0.
dose (cm**(-2)?
1.e15
reading from input file p1hd.1D1
input file p1hd.1D1 closed
writing to output file p1hdrange.dat
output file p1hdrange.dat closed

Additionally: calculation of the damage (or amorphization) probability:

prof1z.exe
program prof1z
input data file?
(not more than 12 ASCII characters)
p1hd.1D1
output data file?
(not more than 14 ASCII characters)
p1hdopt5.dat
options:
iopt
1 range profile
2 nuclear energy deposition
3 electronic energy deposition
4 damage concentration (only valid in c-Si)
5 damage probability (only valid in c-Si)
iopt?
5
backscattering yield (see file "name.OUT")?
0.
atomic density of the single-crystalline substrate
in Angstroem**-3 (see ARHO in "name.OUT")?
0.05
dose (cm**(-2)?
1.e15
reading from input file p1hd.1D1
input file p1hd.1D1 closed
writing to output file p1hdopt5.dat
output file p1hdopt5.dat closed

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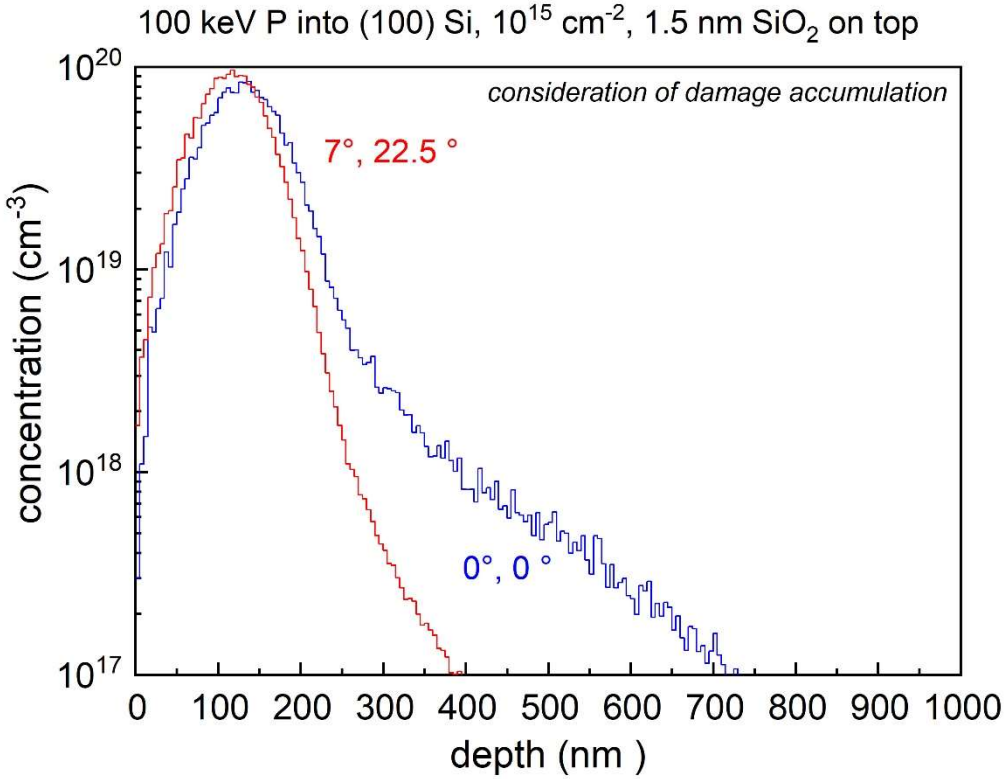
Graphical representation of P depth profiles for Examples E and F

The first diagram shows the P depth profiles p1hcrange.dat and p1hdrange.dat. The diagram differs considerably from that for p1harange.dat and p1hbrange.dat (Examples C and D), which demonstrates that damage accumulation cannot be neglected if the dose is 10^{15} cm^{-2}. The second diagram depicts the depth profile of the damage (or amorphization) probability (p1hcopt5.dat and p1hdopt5.dat). Probability 1 means amorphization. In this manner the depth of the amorphized layer can be determined.



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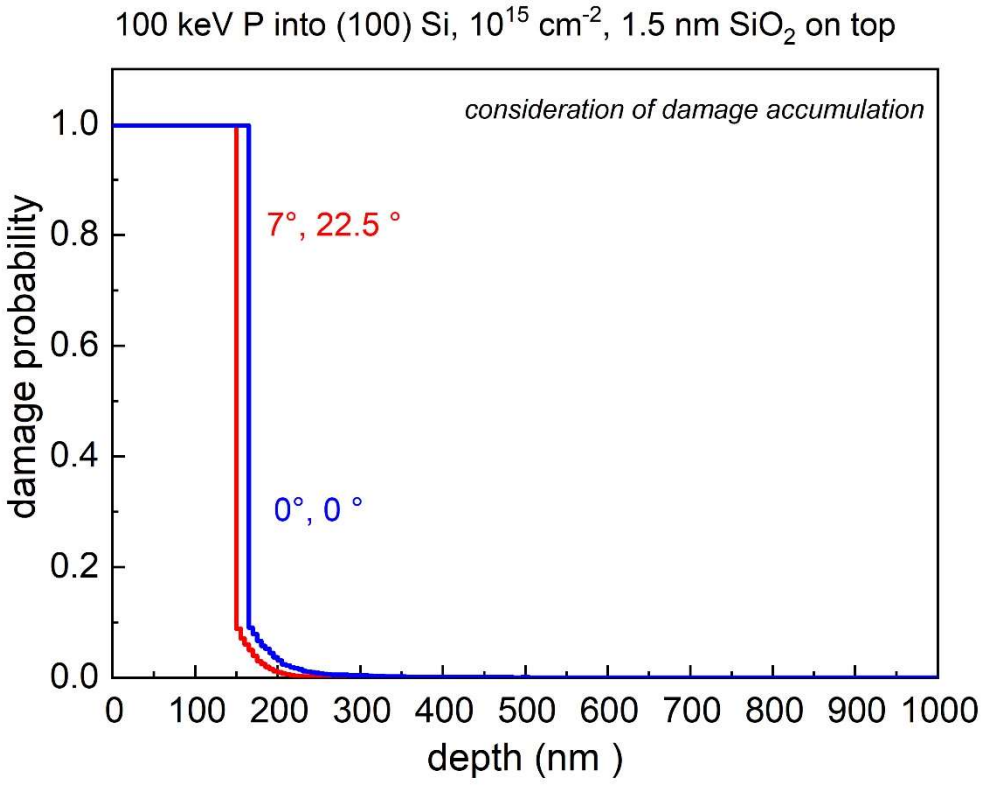

Example G
75 keV ^{116}Sn into (100) diamond, 10^{10} cm^{-2}, 0° tilt, 0° rotation

Step 1: Input dialog using the program xtru04.exe

xtru04.exe

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(C) Since 1991 by
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Input Dialog

File names consist of a variable first part
and a constant second part.
Name of the first part?(exactly 4 ASCII characters!)
s75a
substrate:
single-crystalline Si (1)?

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single-crystalline Ge (2)?
diamond (3)?
3
Ion
Energy in keV?
75
Orientation of the substrate surface (e.g. 1 0 0) ?

Insert a space between the integers!
Please note: Only (100),(110) and (111) surfaces can
be considered!
1 0 0
Tilt angle theta0 in deg.?
0
Rotation angle phi0 in deg.)?
0
Name of the file which contains the parameters
for ZBL electronic stopping?
scoef1.dat - original ZBL 1985 (1)
scoef2.dat - 1989 (2)
scoef1.dat = default in previous Crystal-TRIM applications
1
Atomic (1) or molecular (2) ion?
1
Atomic number?
50
Mass: most abundant isotope (1), another (2)
2
Mass number?
116
clambda is 0.900

use this standard value (yes 1, no 2)?
1
Cel and Cel110 different from 1? (no 1, yes 2)
1
Number of ion histories to be simulated?
10000
Use of an efficient splitting procedure
to improve the statistical precision (no 1, yes 2)?
Splitting is particularly recommended in cases
where long channeling tails are expected.
1
Number of amorphous layers on top of
the single-crystalline substrate (Max.:10):
0
Crystalline substrate:
Temperature different from RT (300K)? (no 1, yes 2)
1
Consideration of damage accumulation
(phenomenological models)? (no 1, yes 2)
1
Width of the intervals in the histograms (A)?
Maximum number of depth intervals is 400
25
Final energy in the simulation of

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```
  the motion of the ions?
   Estimation:
    E(keV)        Range(A)
    0.375E+00     0.657E+01
   Final energy in the simulation of
   the motion of the ions (keV)?
0.375
       writing to input file     s75a.DAT
```

The input data files s75a.IN and s75a.DAT have been written.

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

xtr041.exe < s75a.IN

```
       start in981
       reading from input file     s75a.DAT
       input file closed
       end in981
       start sec971
       end sec971
       start pro981
 status of calculation in %    particle histories
          10                  1000
          20                  1999
          30                  2998
          40                  3997
          50                  4996
          60                  5995
          70                  6994
          80                  7993
          90                  8992
         100                   9991
       end pro981
       start out981
       writing to output file     s75a.OUT
       writing to output file     s75a.1D1
       output file   s75a.1D1        closed
       output file   s75a.OUT        closed
       end out981
```

The output data files s75a.OUT, s75a.1D1 and s75a.ST have been written. Only s75a.1D1 is relevant for following postprocessing.

Step 3: Postprocessing using prof1z.exe

pro1fz.exe

```
            program prof1z
            input data file?
            (not more than 12 ASCII characters)
s75a.1D1
```


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```
            output data file?
            (not more than 14 ASCII characters)
s75arange.dat
               options:
               iopt
               1       range profile
               2       nuclear energy deposition
               3       electronic energy deposition
               4       damage concentration (only valid in c-Si)
               5       damage probability (only valid in c-Si)
      iopt?
1
      backscattering yield (see file "name.OUT")?
0.
      dose (cm**(-2)?
1.e10
      reading from input file     s75a.1D1
      input file   s75a.1D1        closed
      writing to output file     s75arange.dat
      output file   s75arange.dat    closed
```

Additionally: calculation of the "damage concentration", i.e. of the concentration of the ballistically displaced atoms (formation of vacancies and self-interstitials):

```
            program prof1z
            input data file?
            (not more than 12 ASCII characters)
s75a.1D1
            output data file?
            (not more than 14 ASCII characters)
s75aopt4.dat
               options:
               iopt
               1       range profile
               2       nuclear energy deposition
               3       electronic energy deposition
               4       damage concentration (only valid in c-Si)
               5       damage probability (only valid in c-Si)
      iopt?
4
      backscattering yield (see file "name.OUT")?
0.
      dose (cm**(-2)?
1.e10
      reading from input file     s75a.1D1
      input file   s75a.1D1        closed
      writing to output file     s75aopt4.dat
      output file   s75aopt4.dat     closed
```


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Example H
75 keV ^{116}Sn into (100) diamond, 10^{10} cm^{-2}, 7° tilt, 22.5° rotation

Step 1: Input dialog using the program xtru04.exe

xtru04.exe

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Helmholtz-Zentrum Dresden-Rossendorf
Institute of Ion Beam Physics and
Materials Research
Bautzner Landstr. 400
D-01328 Dresden, Germany

Input Dialog

File names consist of a variable first part
and a constant second part.
Name of the first part?(exactly 4 ASCII characters!)
s75b
substrate:
single-crystalline Si (1)?
single-crystalline Ge (2)?
diamond (3)?
3
Ion
Energy in keV?
75
Orientation of the substrate surface (e.g. 1 0 0) ?

Insert a space between the integers!
Please note: Only (100),(110) and (111) surfaces can
be considered!
1 0 0
Tilt angle theta0 in deg.?
7
Rotation angle phi0 in deg.)?
22.5
Name of the file which contains the parameters
for ZBL electronic stopping?
scoef1.dat - original ZBL 1985 (1)
scoef2.dat - 1989 (2)
scoef1.dat = default in previous Crystal-TRIM applications
1
Atomic (1) or molecular (2) ion?
1
Atomic number?

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50
Mass: most abundant isotope (1), another (2)
2
Mass number?
116
clambda is 0.900

use this standard value (yes 1, no 2)?
1
Cel and Cel110 different from 1? (no 1, yes 2)
1
Number of ion histories to be simulated?
10000
Use of an efficient splitting procedure
to improve the statistical precision (no 1, yes 2)?
Splitting is particularly recommended in cases
where long channeling tails are expected.
2
Measure of the statistical precision of simulation
results: ISIGDEPTH?
20
Number of amorphous layers on top of
the single-crystalline substrate (Max.:10):
0
Crystalline substrate:
Temperature different from RT (300K)? (no 1, yes 2)
1
Consideration of damage accumulation
(phenomenological models)? (no 1, yes 2)
1
Width of the intervals in the histograms (A)?
Maximum number of depth intervals is 400
25
Final energy in the simulation of
the motion of the ions?
Estimation:
E(keV) Range(A)
0.375E+00 0.657E+01
Final energy in the simulation of
the motion of the ions (keV)?
0.375
writing to input file s75b.DAT

The input data files s75b.IN and s75b.DAT have been written.

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

xtr041.exe < s75b.IN

start in981
reading from input file s75b.DAT
input file closed
end in981
start sec971

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```
        end sec971
        start pro981
 status of calculation in %    particle histories
           10                  1000
           20                  1999
           30                  2998
           40                  3997
           50                  4996
           60                  5995
           70                  6994
           80                  7993
           90                  8992
          100                   9991
        end pro981
        start out981
        writing to output file     s75b.OUT
        writing to output file     s75b.1D1
        output file   s75b.1D1         closed
        output file   s75b.OUT         closed
        end out981
```

The output data files s75b.OUT, s75b.1D1 and s75b.ST have been written. Only s75b.1D1 is relevant for following postprocessing.

Step 3: Postprocessing using prof1z.exe

pro1fz.exe

```
program prof1z
              input data file?
              (not more than 12 ASCII characters)
s75b.1D1
              output data file?
              (not more than 14 ASCII characters)
s75brange.dat
                 options:
                 iopt
                 1       range profile
                 2       nuclear energy deposition
                 3       electronic energy deposition
                 4       damage concentration (only valid in c-Si)
                 5       damage probability (only valid in c-Si)
        iopt?
1
        backscattering yield (see file "name.OUT")?
0.
        dose (cm**(-2)?
1.e10
        reading from input file     s75b.1D1
        input file   s75b.1D1         closed
        writing to output file     s75brange.dat
        output file   s75brange.dat    closed
```


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Additionally: calculation of the "damage concentration", i.e. of the concentration of the ballistically displaced atoms (formation of vacancies and self-interstitials):

```
            program prof1z
            input data file?
            (not more than 12 ASCII characters)
s75b.1D1
            output data file?
            (not more than 14 ASCII characters)
s75bopt4.dat
              options:
              iopt
              1      range profile
              2      nuclear energy deposition
              3      electronic energy deposition
              4      damage concentration (only valid in c-Si)
              5      damage probability (only valid in c-Si)
      iopt?
4
      backscattering yield (see file "name.OUT")?
0.
      dose (cm**(-2)?
1.e10
      reading from input file     s75b.1D1
      input file   s75b.1D1        closed
      writing to output file     s75bopt4.dat
      output file   s75bopt4.dat     closed
```

Graphical representation of P depth profiles for Examples G and H

The following two diagrams show the Sn depth profiles s75arange.dat and s75bdrange.dat, with a logarithmic and a linear concentration scale. The statistics of the histograms can be improved using simulation with more than 10000 projectile histories.

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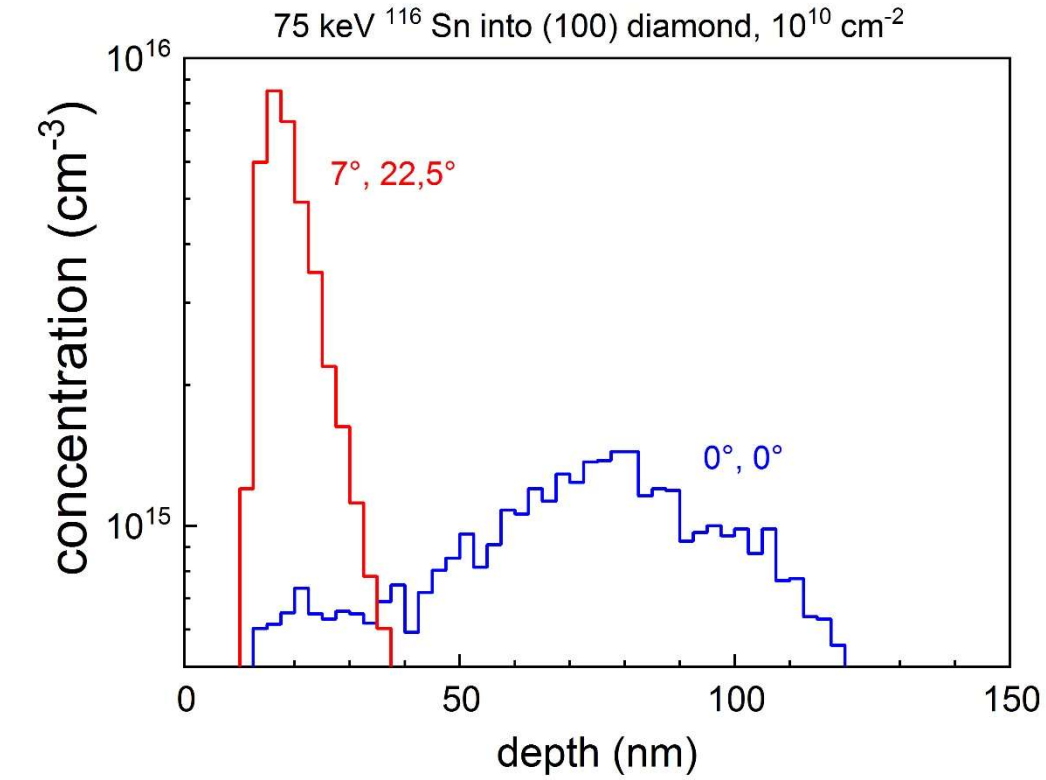

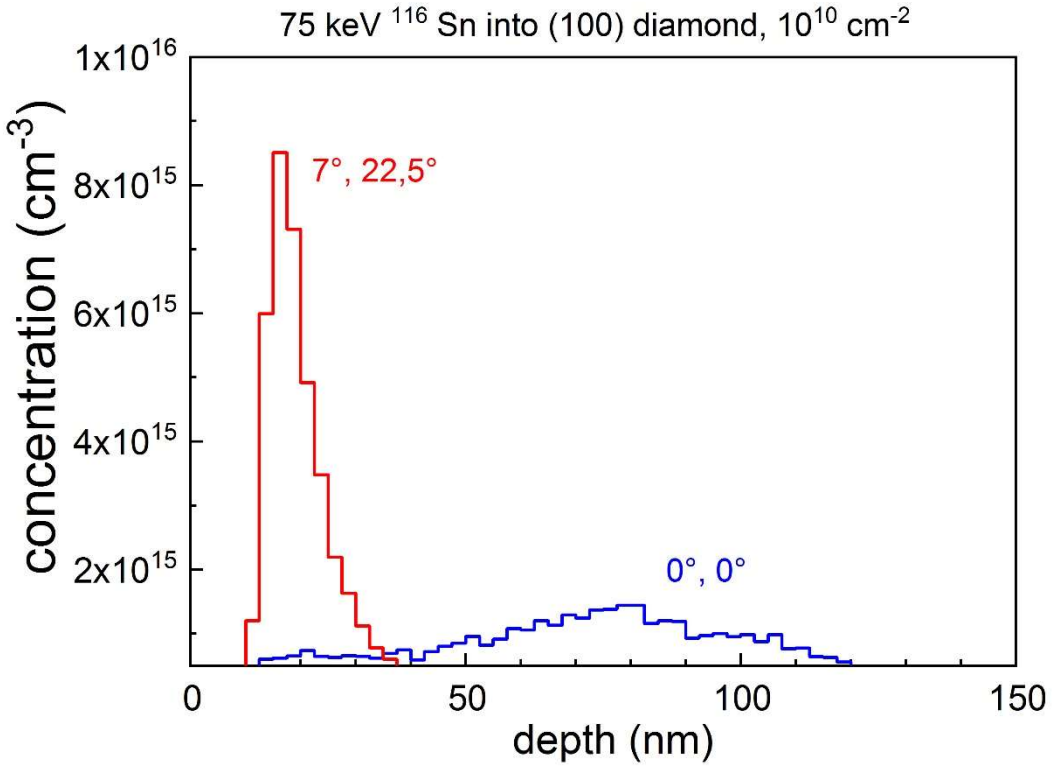

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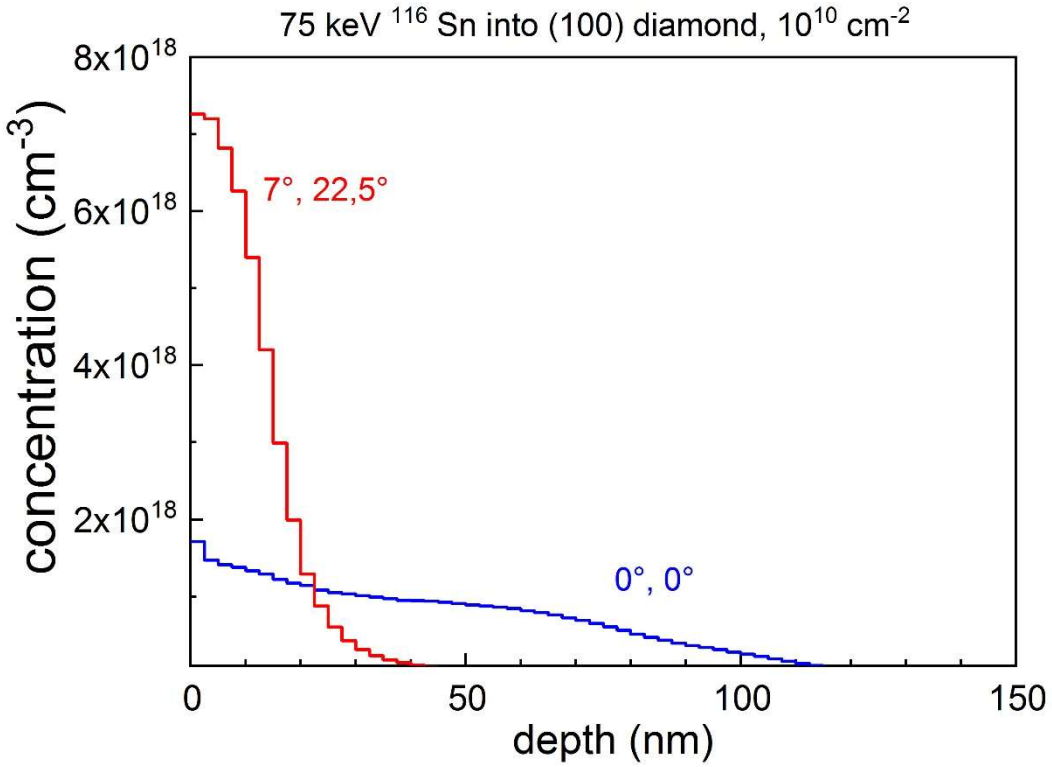
The following diagram shows the concentration of the ballistically displaced atoms.



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