

9 - TRIM: Output Files *

The output of TRIM can be viewed in plots (while the calculation is proceeding) and also in detailed numerical files. The plots are especially useful to see if the calculation is proceeding as expected, but are usually limited in resolution. Most of the datafiles can be requested in the Setup Window for TRIM (menus at the bottom of the window) or can be requested during the calculation. All calculated averages are made over the entire calculation, regardless of when they are requested. That is, if you request a plot of ion ranges after the 100th ion, it will include all the previous ions. Other types of datafiles show details of each ion's interactions, and are started with the file is selected, and continues filing data on each following ion until the file is stopped. If you leave the plots or datafiles "live" during a calculation, they may significantly slow down TRIM.

Chapter Contents

9 - TRIM: Output Files	9-1
Brief Summary of TRIM Plots and Data Files	9-2
<i>Ion/Recoil Distribution Plots and Files:</i>	9-2
<i>Target Damage Plots and Files:</i>	9-3
<i>Full Calculation Details (Datafile COLLISON.txt)</i>	9-3
Ion / Target Example used for Chapter's Output Plots and Files	9-4
Ion Range Distribution and Recoil Atom Distributions.....	9-9
<i>3-Dimensional Ion Range Distributions</i>	9-13
<i>Datafile of Ion Trajectory and Energy in the Target</i>	9-14
<i>Lateral Ion Range Distribution</i>	9-15
<i>3-D plots of the Ion's Electronic Energy Loss</i>	9-17
Backscattered Ions	9-18
Transmitted Ions	9-20
Sputtered Target Atoms	9-21
Combined Tables of Backscattering, Transmitted and Sputtering	9-24
<i>Ion's Energy Loss to the Target Electrons</i>	9-25
<i>Ion's Energy Loss to the Target Phonons</i>	9-26
<i>Energy Loss to Vacancy Production / Replacement Collisions</i>	9-27
<i>Energy Loss from Ions – Energy Loss Absorbed by Target Atoms</i>	9-31
Details of the Ion-Atom Collision Kinetics	9-33
Physics of Recoil Cascades.....	9-33
<i>COLLISON.txt - Type "A"– Ions and Quick Estimate of Damage</i>	9-35
<i>COLLISON.txt - Type "B"– Ions and Recoil Atoms (no cascade data)</i>	9-36
<i>COLLISON.txt - Type "C"– Ions, Recoil Atoms and Cascades</i>	9-38
Special Commands for a TRIM Calculation.....	9-39
<i>Changing TRIM Parameters during the Calculation</i>	9-39
<i>Changing TRIM Plots and Colors (TRIM.cfg)</i>	9-40
<i>Making TRIM Animated Plots</i>	9-40
<i>TRIM "Help, FAQ and Scientific Explanations"</i>	9-41

* Note: This text is Chapter 9 of the SRIM textbook (2008):

“SRIM – The Stopping and Range of Ions in Matter”

Note that TRIM can be stopped during the calculation, and basic parameters may be changed. This allows the user to focus the calculation on a specific problem without having to start over. To change TRIM during a calculation, click on the button ***Pause TRIM*** at the top of the TRIM Calculation window. Then press ***Change TRIM***. All the parameters that can be changed will have a yellow background, and it includes almost all Setup parameters. Make changes in the parameters, or in the colors used for the plots (clicking on the colors in the Target Data window will bring up a color-chart to use). When you are done, press ***End Edit*** and then ***Continue***. This procedure allows the user to modify a TRIM calculation simply, or to superimpose several calculations.

Brief Summary of TRIM Plots and Data Files

<p><i>Note: All TRIM output datafiles are found in the sub-directory: ../SRIM Outputs</i></p>
--

Ion/Recoil Distribution Plots and Files:

- ***Ion Distribution*** : Both Plots and Datafiles are available. The ***Ion Distribution*** plot shows the ion distribution for all ions stopped within the target viewing window. (The ***Viewing Window*** is explained in Chapter 8) and its four statistical moments: range, straggling, skewness and kurtosis (see Chapter 8 for definitions of these moments). These moments are calculated for the entire target (not just the viewing window). The plot ordinate units are $(atoms/cm^3)/(atoms/cm^2)$. When this plot is multiplied by the ion dose (some authors call it a *fluence*) in units of $(atoms/cm^2)$ the plot is directly converted to a target density $(atoms/cm^3)$. See Figure 9-2 for a sample plot, and Table 9-3 and Table 9-4 for sample datafiles.
- ***Ion/Recoil Distribution***: Both Plots and Datafiles are available. The ***Ion/Recoil Distribution*** shows both the ion distribution and all target atom redistributions within the target window. See Figure 9-3 for a sample plot, and Table 9-3 and Table 9-4 for sample datafiles.
- ***Ion Ranges 3D***: Only datafiles are available. Some special applications require detailed 3-D data on the final position of each ion. This is an ACTIVE file, that stores the final three dimensional position of every ion while the calculation is proceeding. A new data line is appended to this file after each ion is finished. No data is recorded until the “***Ion Ranges (3-D data)***” is pressed in the TRIM Calculation Window. Data is then recorded until this box is cleared, or when the calculation ends. See example in Table 9-5.
- ***Ion Trajectory and Energy - 3D***: A datafile may be made of the ion’s position at various energies as it penetrates into the target. See example in Table 9-6. Also included is the electronic energy loss of the ion at that point, and the energy transferred in its last collision. This file allows later plotting of each ion’s trajectory and also a 3D file of the electronic energy loss of each ion.
- ***Ion Lateral Distribution***. Both Plots and Datafiles are available. As the beam penetrates the target, it spreads out. This lateral spread is evaluated for its first and second moments (the same idea as for the 4 moments of the ion range). See Figure 9-5 for a sample plot, and Table 9-7 for a typical datafile.

Ion Backscattering and Transmission Files

- ***Ion Backscattering*** - Some ions might have a strong collision near the surface of the target and may be backscattered back out of the surface of the target. These ions and their kinetic data (final energy and trajectory) can be found in the file ***BACKSCAT.txt*** which is shown in Table 9-9. There is no plot for this data.
- ***Transmitted Ions*** - Some ions reach the bottom of the target and exit through this surface.

These ions, and their kinetic data (final energy and trajectory) can be found in the file **TRANSMIT.txt** which is shown in Table 9-10. There is no plot for this data.

Target Sputtering Files

Ions can cause large cascades of recoil atoms, and their motion may make some of the target recoils exit back through the target surface. These atoms that leave the target surface are called *sputtered atoms*. The number of these atoms may be quite large, and they are often described in a *sputtering yield*, which is defined as the number of atoms sputtered per incident ion. See Figure 9-6 and Figure 9-7. Heavy energetic ions in light targets may cause large sputtering yields- an example is shown in the TRIM Demo “*Se in GaAs*” where the sputtering yield is about 4 target atoms sputtered per incident ion. The value of the sputtering yield is shown in the TRIM Calculation window during the calculation. Files of the energy and trajectory of sputtered atoms can be generated by checking the box “Sputtered Atoms” in either the TRIM Setup window or the TRIM Calculation window. An example of the data file **SPUTTER.txt** file is shown in Table 9-11 and Table 9-12.

Target Damage Plots and Files:

TRIM is often used to gain an understanding of the changes to the target under bombardment by ions. TRIM can be used for detailed examination of this target damage, but it must be interpreted with knowledge of two major TRIM limitations: (a) There is no build-up of ions or damage in the target. Every ion is calculated with the assumption of **zero dose**, i. e. the target is perfect and previous ions have no effect on subsequent ions. (b) The target temperature is 0°K, and there are no thermal effects changing the distribution of ions (thermal diffusion) or affecting the target damage (thermal annealing). Several experiments have been reported at very low temperatures (15 - 40°K) which validate the TRIM results, but show that thermal effects can be quite substantial. For example, for a low dose of ions into crystalline silicon, more than 99% of the target damage may anneal at room temperature. See Chapters 7 and 8 for extended discussions of the various types of damage.

- ***Ion’s Energy Loss to Electrons in the Target*** – Both Plots and Datafiles are available. When ions penetrate into the target, they interact immediately with the target electrons, both single electrons and collectively. This interaction is very complicated, and TRIM uses the physics described in Chapter 3. The energy loss to electrons is collected for the TRIM Viewing Window (in 100 channels of information) and can be accessed during the calculation by selecting the ***Ionization Plot*** button, or the ***Ionization File*** button. The term “Ionization” is often used as a synonym for energy loss to electrons. Examples are shown in Figure 9-8 and Table 9-14. See also the above discussion of Table 9-6.
- ***Ion’s Energy Loss to Phonons in the Target*** – Both Plots and Datafiles are available. See Figure 9-9 and Table 9-15.
- ***Production of Vacancies in the Target.*** – Both Plots and Datafiles are available. See Figure 9-10 and Table 9-16.
- ***Production of Replacement Collisions in the Target.*** – Both Plots and Datafiles are available. See Figure 9-12 and Table 9-17.

Full Calculation Details (Datafile COLLISON.txt)

Almost every detail of the ion’s penetration into the target can be put into a special datafile, ***..SRIM Outputs/COLLISON.txt***, for later examination. This kind of file has various filters available to allow only special details to be recorded. See the later discussion in this chapter on “*Details of the Ion-Atom Collision Kinetics*”.

To get the most detailed file on ion interactions and all the recoil cascades, in the TRIM Setup window select “*Monolayer Collision Step*” in the Damage menu in the upper-right corner. Then check “Collision Details” in the same TRIM Setup window, at the bottom. When a sub-menu comes up and asks if details of the Recoils should also be kept, answer “Yes”.

This selection will overwhelm you with data. For the only the first 5 ions of the ion/target used in this chapter for an example (see Figure 9-1), TRIM will generate 94,000 numbers concerning 12,000 collisions. TRIM provides various filters to help you to screen this data. For example, if you are mostly interested in sampling the ion’s impact on the target, change your TRIM Setup selection from “*Monolayer Collision Step*” to “*Detailed Calculation with Full Damage Cascades*”, and the output datafile drops by 10% to 11,000 collisions. This is because TRIM now uses the Free Flight Path assumption. To further filter the data, if you care mostly about how the ion affects the targets, and you can ignore the recoil cascades, then when you are in the TRIM Setup window, select “Collision Details” and when the sub-menu asks to store data about the recoils, answer “No”. This will reduce the *COLLISON.txt* output for the first 5 ions by 90%, down to about 1,100 collisions.

Ion / Target Example used for Chapter’s Output Plots and Files

In most of the following examples, the calculation will be one of the TRIM Demo Examples available from the TRIM Setup window. This Demo example is a beam of Boron at 200 keV, into a three layer target, see Figure 9-1.

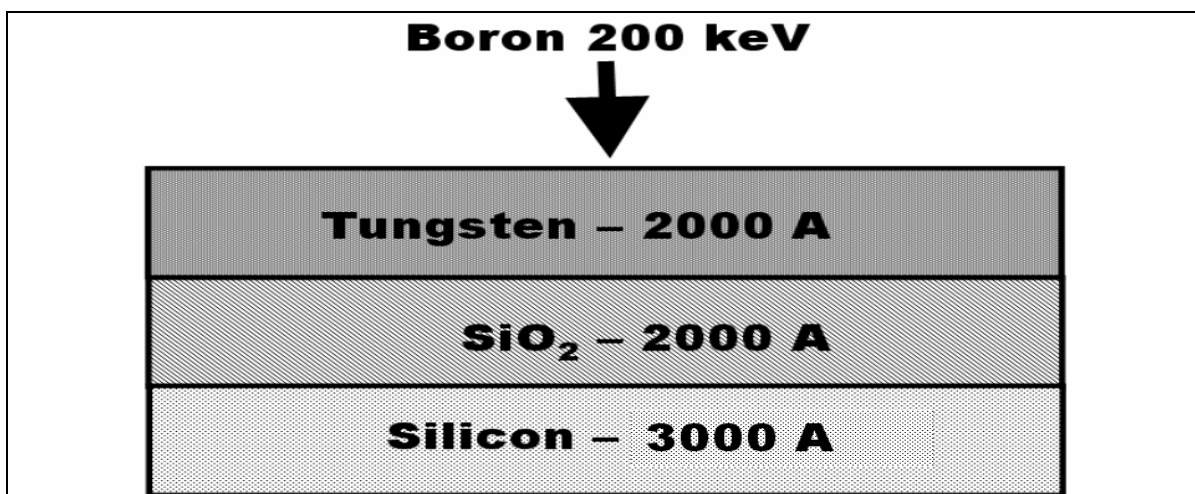


Figure 9-1 SRIM setup for Plots and Output Files

SRIM Demo example of B (200 keV) into a three layer target of W (2000 Å) + SiO₂ (2000 Å) + Si (3000 Å). This setup will be used for most of the examples shown in this chapter.

When you save plots or data files, it is often useful to save the datafile that contains all the details of the calculation. This file can be found in two places in the SRIM directory. The original TRIM Setup data is in the file TRIM.IN, located in the root SRIM direction, Table 9-1. The datafile TRIM.IN is also described in some detail in Chapter 8. Once you start a TRIM calculation, another version is at: *../SRIM Restore/TDATA.sav*, Table 9-2. This file contains all the details of the TRIM calculation, and will include any changes you made to the ion/target parameters during the calculation. This file is created when you stop TRIM and store the results for later use.

Table 9-1 – TRIM.IN contains the Setup parameters for TRIM

```

====> SRIM-2008.01 This file controls TRIM Calculations.
Ion: Z1 , M1, Energy (keV), Angle,Number,Bragg Corr,AutoSave Number.
      5      11      200      0      20000      0      5000
Cascades (1=No;2=Full;3=Sputt;4-5=Ions;6-7=Neutrons), Random Number Seed
              2              0
Diskfiles (0=no,1=yes): Ranges, Backscatt, Transmit, Sputtered,
                        Collisions(1=Ion;2=Ion+Recoils), Special EXYZ.txt file
              0      0      0      1      0      0
Target material : Number of Elements & Layers
"B into W/SiO2/Silicon (Double Peak) " 4 3
PlotType (0-5); Plot Depths: Xmin, Xmax(A) [=0 0 for Viewing Full Target]
      1      0      300
Target Elements:      Z      Mass(amu)
Atom 1 = W =          74      183
Atom 2 = Si =          14      28
Atom 3 = O =           8      16
Atom 4 = Si =          14      28
Layer   Layer Name /      Width  Density      W(74)  Si(14)  O(8)  Si(14)
Numb.   Description      (Ang)  (g/cm3)   Stoich  Stoich  Stoich  Stoich
  1     "Tungsten"        2000   19.3      1       0       0       0
  2     "SiO@2"           2000   2.33      0      .333    .666    0
  3     "Silicon"         2000   2.32      0       0       0       1
Target layer phases (0=Solid, 1=Gas)
0 0 0
Target Compound Corrections (Bragg)
1 1 1
Individual target atom displacement energies (eV)
      21      22      23      22
Individual target atom lattice binding energies (eV)
      2.1      2.2      2.3      2.2
Individual target atom surface binding energies (eV)
      3.1      3.2      3.3      3.2
Stopping Power Version (1=2006, 0=2006)
0

```

Briefly, TRIM.IN's information is mostly in two-line increments. The first line of each pair is a text explanation and does not contain data, and it is followed by a data line which contains the data values.

The first line of TRIM.IN contains the version number of the SRIM software being used:

```

====> SRIM-2008.01 This file controls TRIM Calculations.

```

The 2nd and 3rd lines contain information about the ion (atomic number, mass, energy and incident angle to the target), the total ions to calculate (20,000), a term called "Bragg Corr" that is not used, and the AutoSave number (the TRIM calculation is automatically saved after this number of ions).

```

Ion: Z1 , M1, Energy (keV), Angle,Number,Bragg Corr,AutoSave Number.
      5      11      200      0      20000      0      5000

```

(Note: Several parameters in TRIM are "unused", which means they are left-over from earlier TRIM versions and are kept as dummy variables so TRIM is compatible with other software.)

The next two lines contain parameters for the calculation: (a) the *Cascades* number declares the type of Damage Calculation (upper right menu of the TRIM Setup window), and (b) a random number seed (use zero to use the default value)

Cascades (1=No;2=Full;3=Sputt;4-5=Ions;6-7=Neutrons), Random Number Seed
2 0

The next two lines contain instructions about any datafiles that should be created when TRIM starts (these datafiles are described in the menu at the bottom of the TRIM Setup window). Note that the explanation line is quite long and is duplicated here as two lines of text. In the data line, a “0” means no file, and a “1” asks that this file be created. The EXYZ parameter may be a number such as 1000 - see the section on this file later in this chapter.

Diskfiles (0=no,1=yes): Ranges, Backscatt, Transmit, Sputtered, Collisions (1=Ion;2=Ion+Recoils), Special EXYZ.txt file
0 0 0 1 0 0

The next data line contains (a) a description of the calculation that will be included in every datafile that is produced by TRIM (must be in quotes), and (b) the number of elements in the target and the number of layers in the target. This latter information is necessary because the TRIM.IN file may have several lines of data depending on the number of elements and layers in the target.

Target material : Number of Elements & Layers
"B into W/SiO2/Silicon (Double Peak) " 4 3

The next data line gives that type of initial plot that TRIM should display (use “0” for no plot), and the depths of the Viewing Window. This window can cover the entire target depth, or it can blow-up a small segment of the target so interactions may be seen with greater detail. To default the Viewing Window to the total target depth, you can use “0 0” as the depths.

PlotType (0-5); Plot Depths: Xmin, Xmax(A) [=0 0 for Viewing Full Target]
1 0 300

The next data lines defines the elements in the target. First is the chemical symbol, then the atomic number and finally the mass of each target atom. The number of lines must agree with the number of target elements declared above. The first 15 characters in each line are ignored (e.g. “Atom 1 = W = ”) and are only included to make the file readable. Only the Z and Mass are used by TRIM. In this example, Si (Z=14) is included twice to allow separate analysis of their recoil distributions.

Target Elements:	Z	Mass (amu)
Atom 1 = W =	74	183
Atom 2 = Si =	14	28
Atom 3 = O =	8	16
Atom 4 = Si =	14	28

The next section describes each layer of the target. Note that the explanations takes up two lines of the TRIM.IN datafile. The “Layer Name” is a description (in quotes) that will appear in all the plots. In order to get subscripts use a “@” symbol as shown below for the SiO₂ layer. You can get a superscript by using the symbol “\$”. If you use one of these in the middle of a layer name, then you can return the lettering to normal size using a “_” character. For example, “Fe@2 O@3” will create “Fe₂O₃” for that layer name. Following the layer name is the layer width (Å), the layer density (g/cm³), and the relative concentration of each of the elements in that layer of the target.

Layer Numb.	Layer Name / Description	Width (Ang)	Density (g/cm3)	W(74) Stoich	Si(14) Stoich	O(8) Stoich	Si(14) Stoich
1	"Tungsten"	2000	19.3	1	0	0	0
2	"SiO@2"	2000	2.33	0	.333	.666	0
3	"Silicon"	2000	2.32	0	0	0	1

The next two lines give the phase state of the layers, i.e. whether each layer is a solid or a gas. This is used to calculate the stopping of the ions because, in general, gases have a higher stopping power than equivalent solids (see Chapter 5).

Target layer phases (0=Solid, 1=Gas) 0 0 0
--

The next two lines give any bonding corrections that need to be applied to the electronic stopping powers of the ion (see Chapter 5). A “1” means no special bonding correction.

Target Compound Corrections (Bragg) 1 1 1

The next section gives the damage parameters for the target layers. Each atom has a Displacement Energy, Binding Energy and Surface Binding Energy for each layer. All energies are in units of eV. If an atom does not appear in one layer, you can input “0” for the required energy. See Chapter 7, “TRIM Theory”, for more details.

Individual target atom displacement energies (eV) 21 22 23 22 Individual target atom lattice binding energies (eV) 2.1 2.2 2.3 2.2 Individual target atom surface binding energies (eV) 3.1 3.2 3.3 3.2

The final input is a declaration of which version of SRIM’s Stopping Powers to use. About every 5 years, the complete stopping theory of SRIM is revisited and all the experimental data of that period is added to the database. Any new ideas on stopping theory are also included. This results in new stopping power concepts, and variations in stopping powers from earlier versions of SRIM. The user is usually given the choice of using the new stopping powers, or an older version, for the first couple of years after a major change.

Stopping Power Version (1=2008, 0=2003) 1

A second file containing all the information of a TRIM calculation is found in:

../SRIM Restore/TDATA.sav, see Table 9-2.

This datafile is created when a TRIM calculation is interrupted, and includes data on the calculation in progress as well as any changes that the user has made to the TRIM parameters after the calculation has started. This file, Table 9-2, begins with the version number of SRIM, and the ID text that you gave to the calculation. It then relates the ion data: Atomic Number = 5 (boron), Mass = 11 amu, Energy = 200 keV, impacting at an angle of 0° to the target (perpendicular incidence).

The next item lists the current status of the calculation. This calculation was stopped at ion number 13,126 of a total of 99,999 requested ions. The calculation had an auto-save every 10,000 ions. This means that for a long calculation, after every 10,000 ions all the calculation is saved so if there is a computer failure, the calculation can be restarted at the point of this last save. The “Save Number” can have any value – it is part of your input in the TRIM Setup window. Finally, the calculation to date had zero transmitted ions (ions that went completely through the target) but there were 772 backscattered boron ions. The next lines start to record details at the instant the calculation was stopped. Most of this data is omitted in Table 9-2 to save space. This file is used when you press the button “Resume Saved TRIM Calc” in the SRIM Setup window. When this

button is selected, TRIM reads the data files of the last calculation, including *../SRIM Restore/TDATA.sav*, and can then resume the calculation from the point that it was last saved.

Table 9-2 -“ *../SRIM Restore/TDATA.sav*” contains Restore data for TRIM

```

=====
                        Saved DATA File for TRIM
                  Changes will Modify Continued TRIM Calculations
=====
TRIM Version Number / Calculation Name
"SRIM-2008.01"      "B into W/SiO2/Silicon (Double Peak)      "
ION DATA:At.Numb, Mass(amu), Energy (keV) , Angle to Target
           5         11.0000  2.0000E+02    00.0
ION NUMB: Current, Total, AutoSave, Transmitted, Backscattered
           13126     99999  10000          0         772
=====

..... Calculation Data Omitted .....

===== TARGET MATERIAL =====
Layer # 1 - Tungsten
Layer # 1 - Bottom Depth=      2.E+03 A
Layer # 1- Density = 6.351E22 atoms/cm3 = 19.3 g/cm3
Layer # 1- W = 100 Atomic Percent = 50 Mass Percent
=====

Layer # 2 - SiO@2
Layer # 2 - Bottom Depth=      4.E+03 A
Layer # 2- Density = 7.015E22 atoms/cm3 = 2.33 g/cm3
Layer # 2- Si = 33.3 Atomic Percent = 23.3 Mass Percent
Layer # 2- O = 66.6 Atomic Percent = 26.6 Mass Percent
=====

Layer # 3 - Silicon
Layer # 3 - Bottom Depth=      7.E+03 A
Layer # 3- Density = 4.989E22 atoms/cm3 = 2.32 g/cm3
Layer # 3- Si = 100 Atomic Percent = 50 Mass Percent
=====

Target energies for target atom = W
  Displacement = 21 eV, Binding = 2.1 eV, Surface = 3.1 eV
Target energies for target atom = Si
  Displacement = 22 eV, Binding = 2.2 eV, Surface = 3.2 eV
Target energies for target atom = O
  Displacement = 23 eV, Binding = 2.3 eV, Surface = 3.3 eV
=====

Depth Range of Tabulated Data=  000000.E+00  -  700000.E-02  Angstroms
=====

Total Ions calculated =  013126
Average Range         =  23697.E-01 Angstroms
Average Straggling    =  13420.E-01 Angstroms
Average Vacancy/Ion   =  94044.E-02
=====

Total Backscattered Ions=  772

```


Ion Range Distribution and Recoil Atom Distributions

Ion Distribution Plots

TRIM can determine the final distribution of ions that are directed into a complex target, like that shown in Figure 9-1. The calculation of the ion distribution can be also tabulated in a datafile on the computer, see Table 9-3 and Table 9-4. The target recoil atom distribution is also shown in Figure 9-3, and the numerical values are also found in Table 9-3 and Table 9-4. The plot and tables show the four moments of the final distribution (for definitions of the statistical terms: Range, Straggle, Skewness and Kurtosis, see Chapter 8 in the section "*TRIM Output: Straggling, Skewness and Kurtosis*").

During a TRIM calculation, when the *Ion Distribution "Plot"* box is checked, a range plot is created, Figure 9-2, showing the distribution of the ions in the target. This plot is updated after each ion. The continuous display of the plot slows down the calculation.

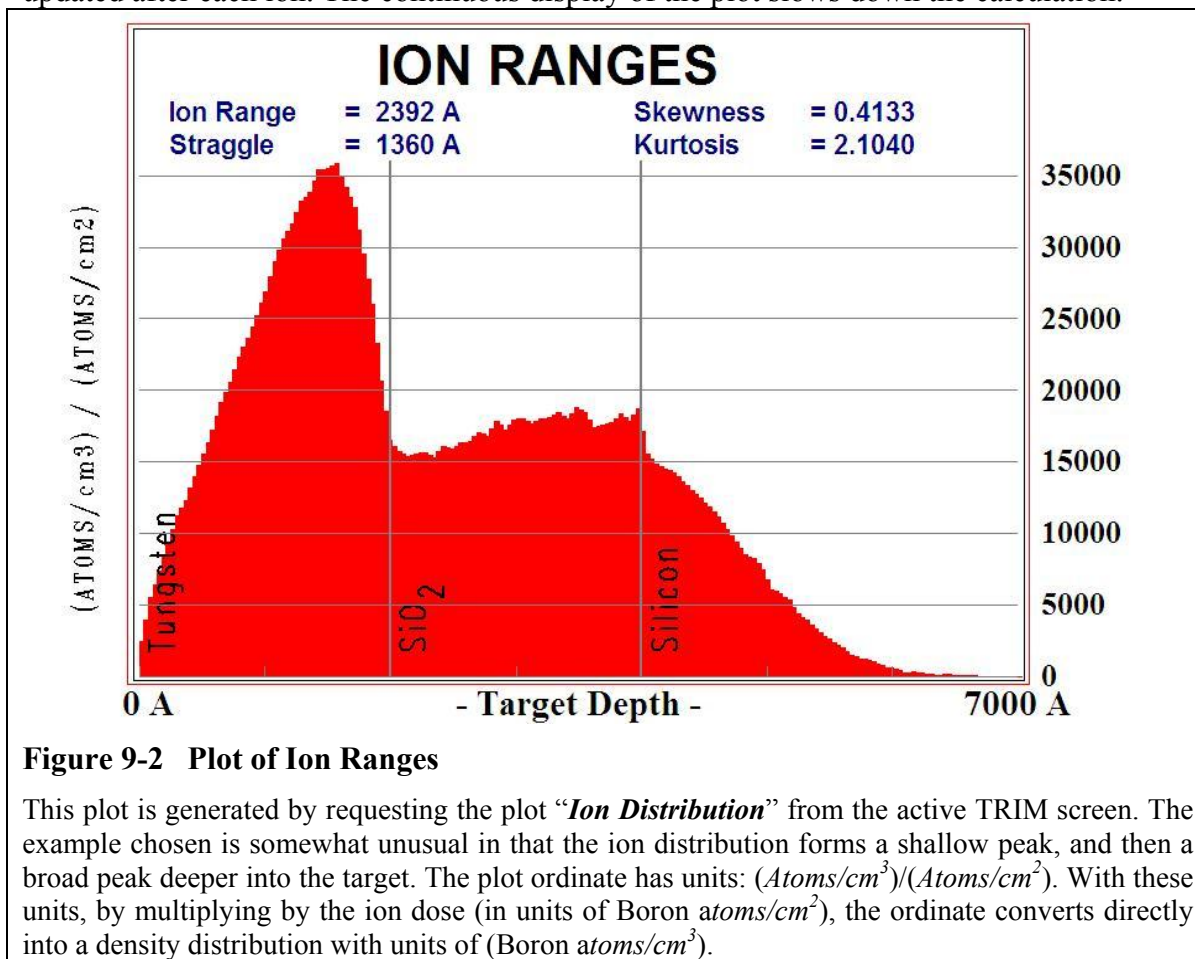


Figure 9-2 Plot of Ion Ranges

This plot is generated by requesting the plot "*Ion Distribution*" from the active TRIM screen. The example chosen is somewhat unusual in that the ion distribution forms a shallow peak, and then a broad peak deeper into the target. The plot ordinate has units: $(\text{Atoms}/\text{cm}^3)/(\text{Atoms}/\text{cm}^2)$. With these units, by multiplying by the ion dose (in units of $\text{Boron atoms}/\text{cm}^2$), the ordinate converts directly into a density distribution with units of $(\text{Boron atoms}/\text{cm}^3)$.

When the *Ion Distribution "File"* button is pressed, a datafile called RANGE.TXT is created (see example below in Table 9-3). This contains the range distribution (final depth) of the ions and all recoiling atoms in the TRIM plot window. The datafile RANGE.TXT is made once, when the button is pressed, and stores the result of the TRIM calculation up to that point in the calculation. (Note: A file which stores the final 3-D coordinates of every ion may be initiated using the separate

check-box called "Ion 3-D Ranges" This option is described later.)

The plot ordinate has units: $(\text{Atoms}/\text{cm}^3)/(\text{Atoms}/\text{cm}^2)$. With these units, by multiplying by the ion dose (in units of Boron atoms/cm²), the ordinate converts directly into a density distribution with units of (Boron atoms/cm³). The word *dose* is sometimes called *fluence*, and is also called the *areal density* of injected ions in units of atoms/cm².

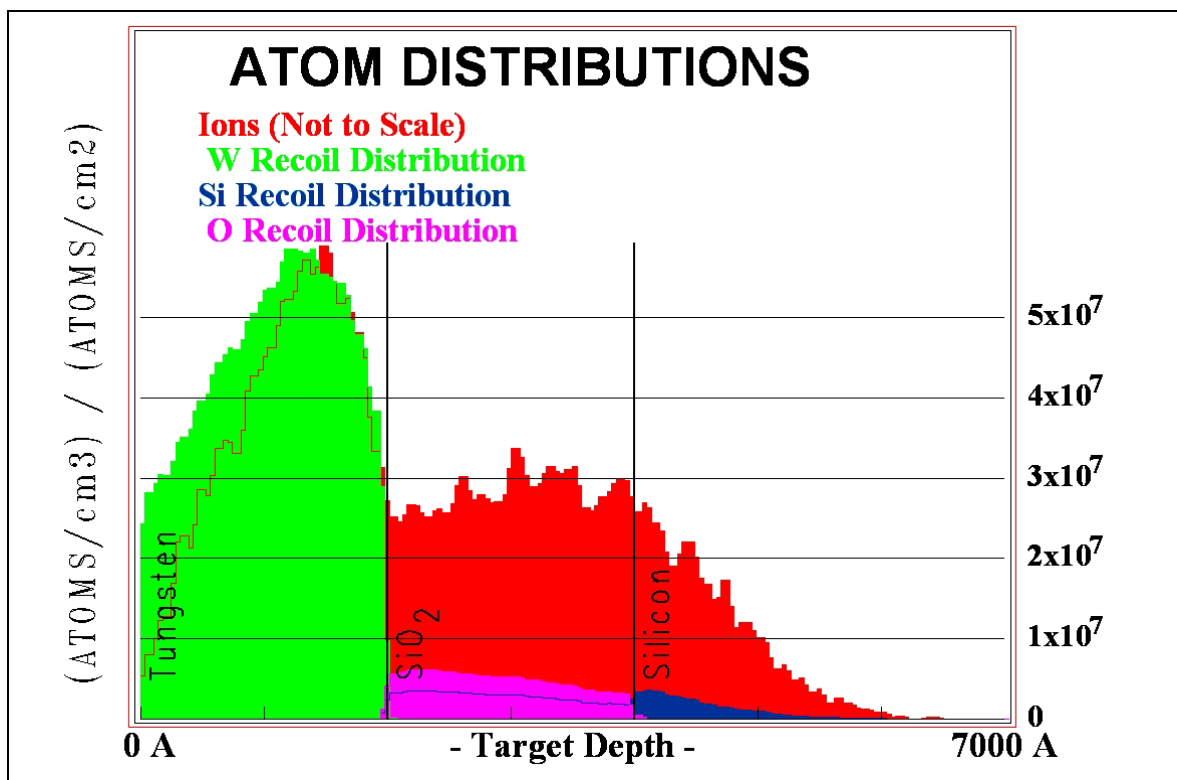


Figure 9-3 Plot of Ion Ranges and Recoil Atom Distributions

This plot is generated by requesting the plot "Ion/Recoil Distribution" from the active TRIM screen. The ion plot is the same shape as shown in Figure 9-2, but scaled to the size of the largest recoil atom plot, and additional plots show the recoil distributions of W, Si and O target atoms. The ion distribution is partially hidden by the large W recoil atoms, and its magnitude is indicated by an outline curve within the W plot. In all cases, there is mixing of the layers, e.g. there are some O atoms that have recoiled into the W layer, but the level is too small to be seen in this plot. Looking at the numerical files, however, O atoms are clearly in the W layer, see Table 9-4. The units of the Ordinate scale are $(\text{Atoms}/\text{cm}^3)/(\text{Atoms}/\text{cm}^2)$, the same as for Figure 9-2. The TRIM calculation window indicates that there are 940 recoil atoms for every incident boron ion. The ion distribution is shown in the figure multiplied by about 1400x so it can be shown on the same plot (see note in plot "Ions - Not to Scale").

When the *Ion Distribution "File"* button is pressed during a TRIM calculation, a datafile called RANGE.TXT is created (see example below in Table 9-3). This file gives various statistical values for the distribution, including mean range, lateral range (width of the distribution), radial range (also width of the distribution using different statistics), straggling, skewness and kurtosis. All of these values are defined in Chapter 8, and also in the HELP beside the button in the TRIM window, and also at the HELP at the top of the TRIM Calculation window by clicking on the button "FAQs and Scientific Explanations". Look for the topic "Statistics of Range Distributions".

Table 9-3 shows the top part of the file *../SRIM Outputs/RANGE.txt*, which includes all the data on the ion and the target, as well as details about the calculation. For the case shown, a total of 13,073 ions were calculated, giving rather accurate ion and atom recoil distributions.

Table 9-3 - RANGE.TXT (File Header Information)

Below is the header at the top of the *../SRIM Outputs/RANGE.txt* file. It contains all the details of the ion, target and the calculation (e.g. a total of 13,073 ions had been calculated for this data).

```

===== B into W/SiO2/Silicon (Double Peak) =====
          SRIM-2006.02
=====
          ION and final RECOIL ATOM Distributions
See   SRIM Outputs\TDATA.txt for calculation details
=====
See file :   SRIM Outputs\TDATA.txt   for details of calculation
Ion       =   B      Energy = 200 keV
===== TARGET MATERIAL =====
Layer  1  : Tungsten
Layer Width=2.E+03A  Layer #1- Density=6.351E22 atoms/cm3 = 19.3 g/cm3
      Layer # 1- W = 100  Atomic Percent = 100  Mass Percent
Layer  2  : SiO2
Layer Width=2.E+03A  Layer #2- Density=7.015E22 atoms/cm3 = 2.33 g/cm3
      Layer # 2- Si = 33.3 Atomic Percent = 46.6 Mass Percent
      Layer # 2-  O = 66.6 Atomic Percent = 53.3 Mass Percent
Layer  3  : Silicon
Layer Width=3.E+03A  Layer #3- Density=4.989E22 atoms/cm3 = 2.32 g/cm3
      Layer # 3- Si = 100  Atomic Percent = 100  Mass Percent
=====
Total Ions calculated =13073.00
Ion Average Range =      236.9E+01 A      Straggling =      134.0E+01 A
Ion Lateral Range =      101.9E+01 A      Straggling =      124.7E+01 A
Ion Radial Range  =      160.0E+01 A      Straggling =      743.3E+00 A
=====
Transmitted Ions =; Backscattered Ions =770
(These are not included in Skewness and Kurtosis below.)
Range Skewness = 000.3955 = [ $\Sigma(X-R_p)^3$ ]/[N*Straggle^3]
Range Kurtosis = 002.1326 = [ $\Sigma(X-R_p)^4$ ]/[N*Straggle^4]
----- Data Omitted from Table -----

```

Table 9-4 shows the bottom part of the file *../SRIM Outputs/RANGE.txt*. It shows the final numerical values for the ions and the recoiling target atoms. The table uses units: $(\text{Atoms}/\text{cm}^3)/(\text{Atoms}/\text{cm}^2)$. With these units, by multiplying by the ion dose (in units of Boron atoms/cm^2), the ordinate converts directly into a density distribution with units of (Boron atoms/cm^3). Note: the word *dose* is sometimes called *fluence*, and it is the *areal density of injected ions* usually in units of Ions/cm^2 .

Table 9-4 contains all the details of the final ion range distribution, and also the final distribution of recoiling target atoms. The table has exactly 100 rows. The target in the SRIM "viewing window" is divided into 100 sub-units. If the target window is 1000A deep, then each row

represents the atoms that end up in each 10Å of the target. For a 10,000Å target, each row would represent 100Å. For the below data, since the target is 7000Å thick, each row is 70Å deep.

It is possible to obtain high depth resolution for a thick target by changing the *viewing window* in the TRIM Setup window. The Viewing window does not have to coincide with the target thickness. For example, in one of the TRIM Demo calculations for “He (5 MeV) in a Gas Ionization Detector” the target is 50mm deep, but the viewing window is only the deepest 10mm, resulting in a range resolution of 0.1mm for tables like Table 9-4.

The plot ordinate has units: $(\text{Atoms}/\text{cm}^3)/(\text{Atoms}/\text{cm}^2)$. With these units, by multiplying by the ion dose (in units of Boron atoms/cm^2), the ordinate converts directly into a density distribution with units of (Boron atoms/cm^3).

Table 9-4- - RANGE.TXT (Ion and Recoil Atom Data Information)

---- Header Data Omitted from Table ----				
=====				
Table Distribution Units are >>> (Atoms/cm3) / (Atoms/cm2)				
=====				
DEPTH (Ang.)	B Ions	W Tgt. Atoms	Si Tgt. Atoms	O Tgt. Atoms
-----	-----	-----	-----	-----
700100.E-04	1.7122E+03	2.0836E+07	0.0000E+00	0.0000E+00
140010.E-03	4.7086E+03	2.8225E+07	0.0000E+00	0.0000E+00
210010.E-03	7.1343E+03	2.9513E+07	0.0000E+00	0.0000E+00
280010.E-03	7.8477E+03	3.0463E+07	0.0000E+00	0.0000E+00
350010.E-03	1.2414E+04	3.3801E+07	0.0000E+00	0.0000E+00
420010.E-03	1.3555E+04	3.5089E+07	0.0000E+00	0.0000E+00
490010.E-03	1.1700E+04	3.7143E+07	0.0000E+00	0.0000E+00
560010.E-03	1.7978E+04	3.9666E+07	0.0000E+00	0.0000E+00
630010.E-03	1.6837E+04	4.0662E+07	0.0000E+00	0.0000E+00
700010.E-03	1.9263E+04	4.3655E+07	0.0000E+00	0.0000E+00
770010.E-03	2.2116E+04	4.6669E+07	0.0000E+00	0.0000E+00
840010.E-03	2.1403E+04	4.5595E+07	0.0000E+00	0.0000E+00
910010.E-03	2.5255E+04	4.9248E+07	0.0000E+00	0.0000E+00
980010.E-03	2.7538E+04	5.0160E+07	0.0000E+00	0.0000E+00
105001.E-02	2.6825E+04	5.3482E+07	0.0000E+00	0.0000E+00
112001.E-02	2.7966E+04	5.3743E+07	0.0000E+00	0.0000E+00
119001.E-02	3.0678E+04	5.4996E+07	0.0000E+00	0.0000E+00
126001.E-02	3.2104E+04	5.7872E+07	0.0000E+00	0.0000E+00
133001.E-02	3.2390E+04	5.7188E+07	0.0000E+00	0.0000E+00
140001.E-02	3.6528E+04	5.7631E+07	0.0000E+00	1.4269E+02
147001.E-02	3.3817E+04	5.8754E+07	0.0000E+00	0.0000E+00
154001.E-02	3.7955E+04	5.4198E+07	0.0000E+00	0.0000E+00
161001.E-02	3.5101E+04	5.5147E+07	0.0000E+00	0.0000E+00
---- Data Omitted from Table ----				

3-Dimensional Ion Range Distributions

The previous section described how to obtain both ion and recoil atom distributions. Many applications require more elaborate 3-Dimensional (3-D) distributions, for example might be an analysis in the semiconductor technology of how implanted ions will spread under a mask edge.

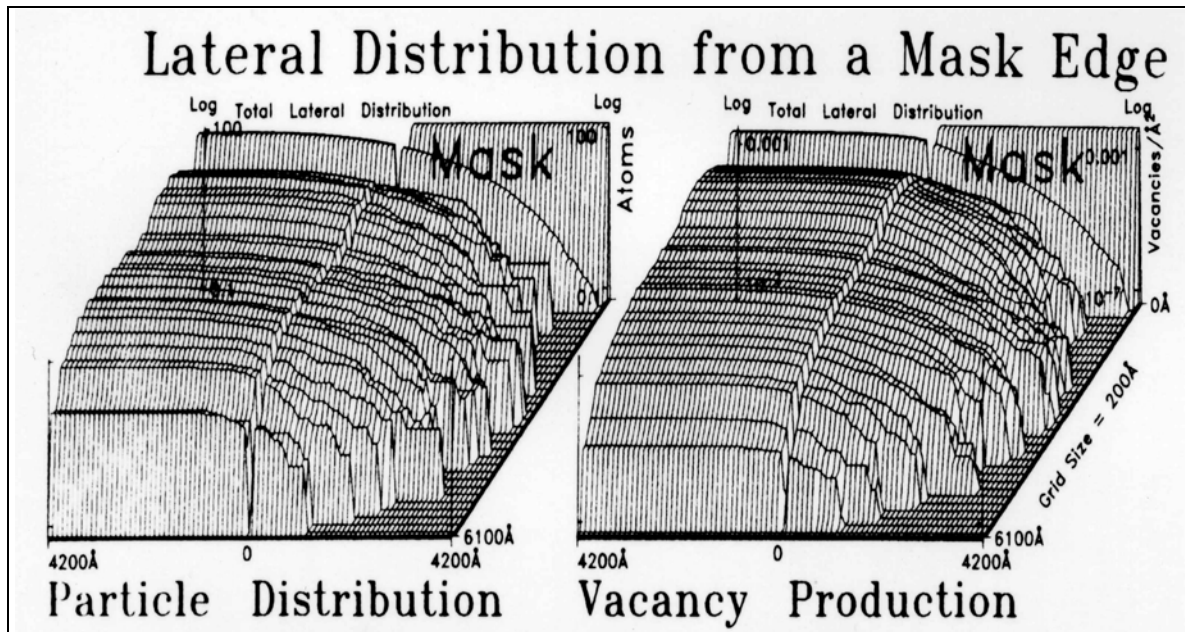


Figure 9-4 – Lateral Distribution of Implanted Ions under a Mask Edge

The figure shows a calculation of the spread of ions under a mask edge. The plot is shown with a boron beam coming into the target described in Figure 9-1. The beam enters from the top of the plot, with the shielding mask (which is assumed to totally absorb the beam that hits it) on the right. There is an artificial line drawn on this isometric plot showing the target directly under the mask edge. The plot's ordinate is shown with a log-scale, so that details of the lateral spread under the mask edge can be seen. An AXIOM of ion implantation is that the impurity concentration directly under a mask edge is exactly $\frac{1}{2}$ of the concentration in an open un-masked area. Novices find this hard to believe, but it is clear that the spread of ions only goes to the right, under the mask, and there are no ions to refill their dilution on the left. So directly under the mask edge the concentration of implanted ions is exactly 50% of that on the far left. The authors have won many a beer using this axiom. (Software to produce the above plot is not included in the SRIM package.)

A 3-D table of ion ranges (with full X,Y,Z coordinates of the final ion position) may be obtained by clicking on the box called “**3-D Ion Ranges**” in the TRIM Calculation window. This data is not stored unless this box is checked, so initiating it starts the storage of the final ion positions from the time the request is made. This datafile is called `../SRIM Outputs/RANGE_3D.txt`, and it will be appended for the remainder of the TRIM calculation until the check mark is removed by clicking on it again.

Shown in Table 9-5 is the table `../SRIM Outputs/RANGE_3D.txt` which contains the final positions of the ions in the target shown in Figure 9-1. Tabulated are ions number 13082-13094. At the top of RANGE_3D.TXT is a description of the calculation. Then the ions are tabulated with their X (depth), Y and Z (lateral) coordinates. Any ions which are backscattered or transmitted are not tabulated (note that backscattered ion #13089 is missing from the table). If the incident ion

beam is specified as at an angle to the target, this angle is in the X-Y plane. See details in Chapter 7 and 8.

This table can then be used to generate special 3-D plots such as shown in Table 9-4 using standard 3-D software (not included in SRIM).

Table 9-5 - RANGE_3D.TXT (Final 3D Ion Distribution)

===== SRIM Outputs\RANGE_3D.txt =====			
Ion = B (05) Ion Mass= 011.0000			
Energy = 2000000.E-04 keV			
Ion Angle to Surface = 00.0 degrees			
---- Header Data Omitted from Table (See Table 9-3) ----			
Ion Number	Depth X (Angstrom)	Lateral Y (Angstrom)	Lateral Z (Angstrom)
-----	-----	-----	-----
0013082	4.4202E+03	1.1992E+03	8.4194E+01
0013083	2.5755E+03	2.2882E+03	4.9715E+02
0013084	1.8796E+03	2.4276E+03	9.7905E+02
0013085	4.1970E+03	5.9111E+02	-1.0712E+03
0013086	3.7087E+03	-1.5715E+03	-2.3427E+03
0013087	2.5107E+03	1.4551E+03	-4.4562E+02
0013088	3.1975E+03	2.5150E+02	2.3512E+03
0013090	3.0767E+03	1.1650E+02	-1.3126E+03
0013091	1.4088E+03	-2.4023E+03	-1.2174E+02
0013092	4.3233E+03	8.1428E+02	-3.8231E+02
0013093	3.2774E+03	-1.3397E+03	6.3019E+02
0013094	1.3404E+03	2.5045E+03	2.0818E+02
---- Data Omitted from Table ----			

Datafile of Ion Trajectory and Energy in the Target

You can track the 3-dimensional position of an ion at intervals through its path into the target. To do this, in the TRIM Setup window, at the bottom, is a window called “**Special EXYZ File Increment (eV)**” For example, assuming an incident ion of 200 keV, if 10000 (eV) is entered as the EXYZ increment, the table will show the ion’s position at 10 keV increments, e.g. at 200 keV, 190 keV, 180 keV,.... The datafile of the ion position will be stored at these specific energies into: *../SRIM Outputs / EXYZ.txt*

An example of the datafile using this command is shown in Table 9-6 for the target of Figure 9-1. The EXYZ parameter is set for 10,000 eV (10 keV), which gives about 20 positions for each ion’s track. The ion energies are not exactly at the 10 keV intervals because the energy losses of the ion occur in uneven steps. The position of the ion at the nearest energy to each increment is used for the table. Note in column 6 is tabulated the electronic stopping power (eV/Å), and in column 7 is the energy lost (eV) to a target atom during the ion’s last ion/target atom collision.

It is possible to setup TRIM for another EXYZ file example using the TRIM Demo for Bi(500 keV) ions into silicon. This DEMO is set so that every time the ion loses 25 keV, an entry will be

made into the file of the Bi ion's position. That is, the ion's position is stored at energies of about 500 keV, 475 keV, 450 keV, 425 keV....

Table 9-6 - Table of 3-D Position of Ion Trajectory and Energy in Target

= Ion Energy vs Position File =						
=====						
= AXIS DEFINITIONS: X=Depth, Y,Z= Lateral plane of target surface.=						
= (If beam enters target at an angle, this tilt is in Y direction)=						
= Shown are: Ion Number, Energy (keV), X, Y, Z Position =						
===== CALCULATION DATA =====						
Ion Data: Name, Mass, Energy, Energy Interval						
B 11.00 200keV 10000eV						
=====						
Ion Number	Energy (keV)	Depth (X) (Angstrom)	Y (Angstrom)	Z (Angstrom)	Electronic Stop. (eV/A)	Energy Lost to Last Recoil (eV)

0000001	2.0000E+02	0.0000E+00	0.0000E+00	0.0000E+00	7.1892E+01	0.0000E+00
0000001	1.8952E+02	1.5127E+02	-7.5751E-01	-1.0005E+00	7.0049E+01	2.2508E+00
0000001	1.7998E+02	2.7998E+02	1.0416E+00	-1.0838E+01	6.8356E+01	2.4354E-01
0000001	1.6847E+02	3.7142E+02	8.0857E+00	-1.9087E+01	6.6291E+01	3.7167E+00
0000001	1.5974E+02	4.7846E+02	2.4859E+01	-3.2319E+01	6.4704E+01	2.0871E+00
0000001	1.4987E+02	5.7549E+02	4.1584E+01	-4.8587E+01	6.2887E+01	5.2197E+01
0000001	1.3997E+02	8.1777E+02	6.6407E+01	-9.5390E+01	6.1027E+01	6.5079E+01
0000001	1.2475E+02	9.8262E+02	7.9988E+01	-1.2718E+02	5.8073E+01	7.0028E+03
0000001	1.1635E+02	1.0987E+03	-7.8480E+01	-1.8039E+02	5.6371E+01	6.4216E+00
0000001	1.0966E+02	1.1916E+03	-2.5511E+02	-2.0275E+02	5.4967E+01	7.1201E+00
---- Data Omitted from Table ----						

Lateral Ion Range Distribution

The range of ions has been described above with regard to the final distribution as a function of depth below the target surface. For ion beams with perpendicular incidence to the target, the ion distribution will spread out with azimuthal symmetry. The spread of ions laterally can be conveniently summarized by using the averaging:

$$\text{Eq. 9-1} \quad \text{Lateral Range} \quad \equiv \quad \Sigma_i |y_i| / N \quad = \quad < |y| >$$

$$\text{Eq. 9-2} \quad \text{Lateral Straggling} \quad \equiv \quad [\Sigma_i ((|y_i| + |z_i|)/2)^2 / N]^{1/2}$$

$$\text{Eq. 9-3} \quad \text{Radial Range} \quad \equiv \quad R_r = \Sigma_i (y_i^2 + z_i^2)^{1/2} / N$$

Where y_i is the final y-axis value of the ion, z_i is the final z-axis value of the ion, and N is the number of ions calculated. Thus the Lateral Range is merely the average final y-z displacement of the ions assuming a perpendicular incidence of the ion beam.

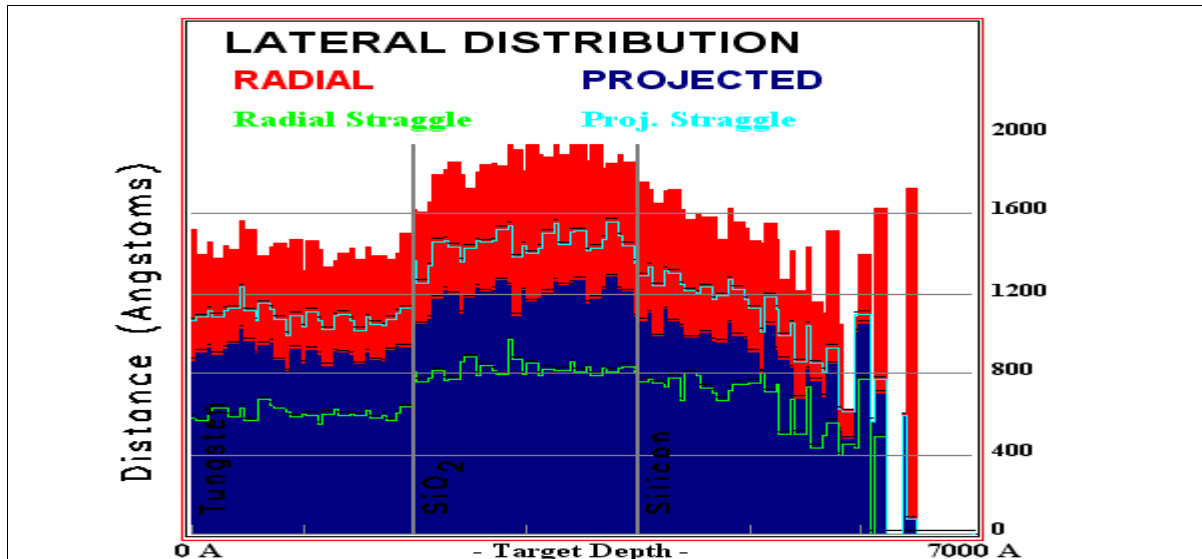


Figure 9-5 - Lateral Spread of Ions

The figure shows the lateral spread of the ions from the original ion axis. Both the first moment of the spread (solid plots) and the second moment, the straggle, of the spread (line plots) are shown. These plots are easier to see on the computer screen where each part is color coded.

The datafile, *../SRIM Outputs/LATERAL.txt* , and the plot summarizes the lateral spread of ions within the target window.

- The plot is created when the TRIM Calculation window button “*Lateral Range*” Plot is pressed, and then this plot is updated after each later ion. The continuous display of the plot slows down the calculation.
- The datafile is created once, when the “*Lateral Range*” File button is pressed (see Table 9-7 below) The datafile summarizes the calculation to that point. Also included in this datafile are averages of both the Range, the Lateral Range and the Radial Range..
- The datafile also includes the extended note:

“NOTE : The Projected LATERAL Spread is based on a projection on a plane - just the way the XY or XZ displays look on the screen. The Lateral Projected Range is defined as the average of the absolute values of the projected lateral displacements from the X-axis. One use of this range: If a mask covers half of a target, the lateral range is the distance under the mask where the concentration drops to 25% (at the mask edge the concentration= 50% of the uniform value). The Radial Range is the mean radial displacement range from the X-axis assuming cylindrical symmetry.”

Table 9-7 - LATERAL.TXT (Ion Range Distribution)

===== B into W/SiO2/Silicon (Double Peak) =====				
SRIM-2006.02				
=====				
LATERAL SPREAD OF IONS				
=====				
NOTE : The Projected LATERAL Spread is based on a projection on a plane- just the way the XY or XZ displays look on the screen. The Lateral Projected Range is defined as the average of the absolute values of the projected lateral displacements from the X-axis. One use of this range: If a mask covers half of a target, the lateral range is the distance under the mask where the concentration drops to 25% (at the mask edge the concentration= 50% of the uniform value).				
The Radial Range is the mean radial displacement range from the X-axis assuming cylindrical symmetry.				
=====				
Ion Average Range = 236972.E-02 A Stragglng = 134204.E-02 A				
Ion Lateral Range = 101693.E-02 A Stragglng = 124470.E-02 A				
Ion Radial Range = 159752.E-02 A Stragglng = 742356.E-03 A				
=====				
TARGET DEPTH (A)	LATERAL PROJ.RANGE (Angstroms)	Projected Stragglng (Angstroms)	LATERAL RADIAL (Angstroms)	Radial Stragglng (Angstroms)
7001000.E-05	86047569.E-05	10618028.E-04	15144395.E-04	57437670.E-05
1400100.E-04	90123628.E-05	10804629.E-04	13958601.E-04	56282605.E-05
2100100.E-04	92878883.E-05	11137749.E-04	14525209.E-04	59630276.E-05
2800100.E-04	89000485.E-05	10831485.E-04	13759439.E-04	62767446.E-05
3500100.E-04	91299021.E-05	11041263.E-04	14327649.E-04	62547777.E-05
4200100.E-04	94310302.E-05	11228703.E-04	14184628.E-04	58636979.E-05
4900100.E-04	10303406.E-04	12348963.E-04	15515912.E-04	62491014.E-05
5600100.E-04	94818444.E-05	10952660.E-04	15095818.E-04	55719145.E-05
---- Data Omitted from Table ----				

3-D plots of the Ion's Electronic Energy Loss

Some applications require the generation of three dimensional plots of the electronic energy loss of the ions. Examples of such applications are the use of ion beams for micro-lithography, or the use of ion beams in studying or altering biological samples. One method to do this was discussed before in "*Datafile of Ion Trajectory and Energy in the Target*", see Table 9-6. The steps below generate a more detailed datafile. (Note that this procedure may be inaccurate for heavy ions which create significant recoil cascades. The electronic energy loss of the recoils is omitted.)

- Setup your TRIM target in the usual way.
- Check the box for Collision Details (bottom of setup window).
- Continue with the TRIM setup program. When TRIM starts, you will be asked whether you wish to create a *New* file or *Append* to an old COLLISON.txt file. Specify *New*. Run TRIM for several ions. You will notice that the box called *Collision Details* is checked. You can start this file at any time during the TRIM calculation by checking this box, and stop it by unchecking it later.

- After several ions are completed, stop TRIM
- Now edit the file **COLLISON.txt**. You will see a file like the one shown below:

Table 9-8 - 3-D plots of Ion's Electronic Energy Loss (COLLISON.txt)

TRIM Calc.= B(17 keV)==> Tungsten(300A)												
----- COLLISION HISTORY -----												
NOTES: Only Ion Collisions which produce Displacements are tabulated.												
Atom Sums and Averages are Incomplete if Recoil Cascades Leave Target.												
Target DISplacements = VACancies + REPLACement Collisions.												
Target VACancies = INTERstitial Atoms + (Atoms Leave Target Volume).												
Ion	Energy	Depth	Lateral Dist(A)		Se	Atom	Recoil	Tgt	Tgt	Tgt	Tgt	
Num	(keV)	(A)	Y Axis	Z Axis	(eV/A)	Hit	Engy (eV)	DISP	VAC	REPLAC	INTER	
1	16.00E+00	33E+00	1E-05	4E+00	15.84	W	83E+00	0	0	0	0	
1	16.10E+00	49E+00	-3E-02	7E+00	15.86	W	57E+00	4	2	2	2	
1	16.28E+00	65E+00	-6E+00	6E+00	15.93	W	94E+00	2	1	1	1	
1	16.06E+00	111E+00	-12E+00	-8E+00	15.85	W	48E+00	4	1	3	1	
1	15.00E+00	125E+00	-14E+00	-15E+00	15.32	W	114E+00	2	1	1	1	
----- Data Omitted -----												

This file shows the three-dimensional position of each major collision between the ion and the target atoms. It also shows in column six the instantaneous electronic energy loss of the ion to the target in units of eV/Å. If you need the three-dimensional electronic energy loss of the ion to the target, you now have all the necessary information. To obtain the energy deposited, calculate the path length between two successive collisions and multiply by the specific energy loss. For example, the distance between the first two collisions shown above is 16.3Å, with an energy loss of 15.86 eV/Å. This means the ion loses 258 eV into electronic excitations in this segment. If higher accuracy is needed, one can interpolate between the instantaneous energy loss values shown at each major collision point. Note that electronic stopping, col. 6, does not smoothly change due to Monte Carlo straggling variations.

NOTE that this table does not include the electronic energy loss of recoiling atoms- only that of the ions.

This application was suggested by Lidia Didenko, Univ. of Maryland.

Backscattered Ions

Backscattered ions are those which, after one or more target collisions, have a trajectory that exits the target back through its surface. The datafile **../SRIM Outputs/BACKSCAT.txt** contains the kinetic data of Backscattered Ions. The datafile is opened when the **Backscattered Ions** selection is checked in the TRIM Setup window , or when the **Backscattered Ions** button is pressed in the TRIM Calculation window.

An example is shown in Table 9-9 for the target shown in Figure 9-1. The first 9 lines of BACKSCAT.txt describe the data in this file. Line #10 is a short description of the current calculation based on your input.

Table 9-9 - BACKSCAT.TXT (Backscattered Ions Kinetics)

```

===== SRIM-2006.02 =====
=====
= SRIM Outputs\BACKSCATSRIM Outputs\ : File of Backscattered Ions      =
= This file tabulates the kinetics of ions or atoms leaving the target.  =
= Column #1: S= Sputtered Atom, B= Backscattered Ion, T= Transmitted Ion.=
= Col.#2: Ion Number, Col.#3: Z of atom leaving, Col.#4: Atom energy (eV)=
= Col.#5-7: Last location: X= Depth into target, Y,Z= Transverse axes.  =
= Col.#8-10: Cosines of final trajectory.                                =
= *** This data file is in the same format as TRIM.DAT (see manual)      =
= TRIM Calc.= B(200 keV) ==> Tungsten+SiO2+Silicon( 7000 A)            =
  Ion  Atom  Energy  Depth      Lateral-Position      Atom Direction
  Numb Numb  (eV)    X (A)      Y (A)      Z (A)      Cos (X)  Cos (Y)  Cos (Z)
B   18    5  .15625E+05 -44030E-07 .3389E+03 .1930E+04 -.7723 -.2483 .5846
B   59    5  .73610E+04 -59772E-07 -.1148E+04 -.1856E+04 -.32106 -.8717 .3700
B   60    5  .30068E+05 -10512E-07 .6851E+03 -.8028E+03 -.77827 -.2837 .5601
B   90    5  .95421E+05 -20704E-06 .1986E+02 .4276E+03 -.87273 .0660 .4837
B  103    5  .31129E+05 -19596E-06 -.1222E+04 -.3741E+03 -.96821 .2025 -.1467
B  119    5  .94703E+05 -23078E-06 -.2757E+03 -.1914E+03 -.99243 .1175 .0355
B  127    5  .39248E+05 -14227E-06 -.1143E+04 .1261E+04 -.92518 -.2322 .3001
B  135    5  .11210E+06 -10779E-06 -.2087E+03 .3356E+03 -.65032 -.4227 .6311
B  153    5  .56244E+05 -14285E-06 .3022E+03 .3440E+03 -.89376 .1925 .4050
B  154    5  .70127E+05 -10415E-06 .5957E+02 .1529E+04 -.78766 -.3408 .5132

```

---- Data Omitted from Table ----

For correct Display of this datafile, use Microsoft font "Courier New" or "MS-LineDraw". "Linedraw" is included in the SRIM software package. See the subdirectory: SRIM/Data/Linedraw.ttf

Lines #11 - 12 are descriptive headers to the columns of data. The first column in all the data fields in this table is the letter "B" which indicates that this is a backscattered ion. This letter is also used in the summary file TRIMOUT.dat (see Table 9-13) which includes entries from datafiles BACKSCAT.txt, TRANSMIT.txt and SPUTTER.txt. Next is the sequential ion number starting with #18 (ion numbers 1-17 are not backscattered and are omitted), followed by ion #59. Column #3 is the atomic number of the ion. Column #4 is the energy of the backscattered ion (eV) as it leaves the target. Column #5 is its position when it was declared *backscattered*. Since the target atoms are randomly placed within their lattice cells, this number will vary slightly from zero, but will always be in the upper monolayer of the target. Columns #6-7 are the lateral position of the ion when it exits the target. Columns #8-10 are the directional cosines of the trajectory of the backscattered ion. Note that cos(X) is always negative, since the x-axis measures depth into the target and this indicates a backwards trajectory.

Note that all the data files BACKSCAT.txt, TRANSMIT.txt and SPUTTER.txt (Table 9-9, Table 9-10 and Table 9-11) have the same format, and can be used as input for a subsequent TRIM calculation. This is necessary for some of the special applications discussed in Chapter 8, the TRIM Input chapter.

Transmitted Ions

The plot and the datafile `./SRIM Outputs/TRANSMIT.txt` contains the kinetic data of Transmitted Ions. It contains the kinetic data of Ions which leave the bottom of the target. The datafile is opened when the *Transmitted Ions* selection is checked in the TRIM Setup window, or when the *Transmitted Ions* button is pressed in the TRIM Calculation window.

Table 9-10 - TRANSMIT.TXT (Transmitted Ion Kinetics)

===== SRIM-2006.02 =====									
===== TRANSMIT.txt : File of Transmitted Ions =====									
= File tabulates the kinetics of ions or atoms leaving the target. =									
= Col. #1: S= Sputtered Atom, B= Backscattered Ion, T= Transmitted Ion.=									
= Col.#2: Ion Number, Col.#3: Z of atom leaving, Col.#4: Atom energy)=									
= Col.#5-7: Last location: X= Depth into target, Y,Z= Transverse axes=									
= Col.#8-10: Cosines of final trajectory. =									
= TRIM Calc.= B(300 keV) ==> Tungsten+SiO2+Silicon(7000 A) =====									
	Ion	Atom	Energy	Depth	Lateral-Position			Atom Direction	
	Numb	Numb	(eV)	X(A)	Y(A)	Z(A)	Cos(X)	Cos(Y)	Cos(Z)
T 1	5	.7838E+03	7000E-03	.3092E+03	.3348E+04	.8839	.2127	-.4164	
T 7	5	.2891E+05	7001E-03	.6063E+03	-.1998E+04	.7350	.6451	-.2084	
T 10	5	.1088E+05	7002E-03	.2308E+04	.6435E+03	.9840	-.1623	-.0728	
T 11	5	.9959E+04	7002E-03	.2709E+04	-.4060E+04	.7797	.3948	-.4858	
T 12	5	.1576E+05	7001E-03	.3100E+03	-.1407E+04	.9119	.1164	.3934	
T 13	5	.1432E+05	7001E-03	.1441E+04	.1857E+04	.8282	.5170	.2161	
---- Data Omitted from Table ----									

For correct Display of this file, use Microsoft font "Courier New" or "MS-LineDraw". "Linedraw" is included in the SRIM software package. See the subdirectory: SRIM/Data/Linedraw.ttf

NOTE: Table 9-10 was calculated with the target of Figure 9-1, however the boron ions were set at 300 keV, instead of 200 keV, in order to get some ions transmitted through the target.

The first 7 lines of TRANSMIT.TXT, Table 9-10, describe the data. Line #8 is a short description of the calculation based on your input. Lines #9 - 10 are descriptive headers to the data fields. Beginning in line #11 is the data. The first item in all these data fields is the letter "T" which indicates that this is a transmitted ion (this letter is also used in the summary file TRIMOUT.DAT (see Table 9-13) which includes entries from BACKSCAT.TXT, TRANSMIT.TXT and SPUTTER.TXT.) Next is the sequential ion number (ions number 2-6 are not transmitted). Column #3 is the atomic number of the ion. Column #4 is the energy of the transmitted ion (eV). Column #5 is its position when it was declared *transmitted*. Since the target atoms are randomly placed within their lattice cells, this number will vary slightly from the total target depth of 7000Å. Columns #6-7 are the lateral position of the ion when it exits the target. Columns #8-10 are the directional cosines of the trajectory of the backscattered ion. Note that cos(X) is always positive, since the x-axis measures depth into the target, and cos(x) = 1 would mean a perpendicular exit from the target.

Note that all the data files BACKSCAT.txt, TRANSMIT.txt and SPUTTER.txt (Table 9-9, Table 9-10 and Table 9-11) have the same format, and can be used as input for a subsequent TRIM

calculations. This is necessary for some of the special applications discussed in Chapter 8, the TRIM Manual.

Sputtered Target Atoms

The datafile `../SRIM Outputs/SPUTTER.txt` contains the kinetic data of Sputtered Target Atoms. The datafile is opened when the *Sputtered Atoms* selection is checked in the TRIM Setup window, or when the *Sputtered Atoms* button is pressed in the TRIM Calculation window.

In contrast to files for backscattered or transmitted ions, TRIM maintains a constant file of sputtered atoms and their energy. This is important because the target **Surface Binding Energy** (SBE) is used to determine if a recoiling target atom has enough energy to leave the solid, or whether it will be held in by the target's surface binding energy. These energies are not well known, and the plots allow the user to see what would be the effect of changing this value from that suggested. Among other problems in determining its value, the Surface Binding Energy will change as the target roughens after initial sputtering (its SBE would probably decrease), or materials like silicon crystal will become amorphous with extended bombardment, and the sputtering yield will change.

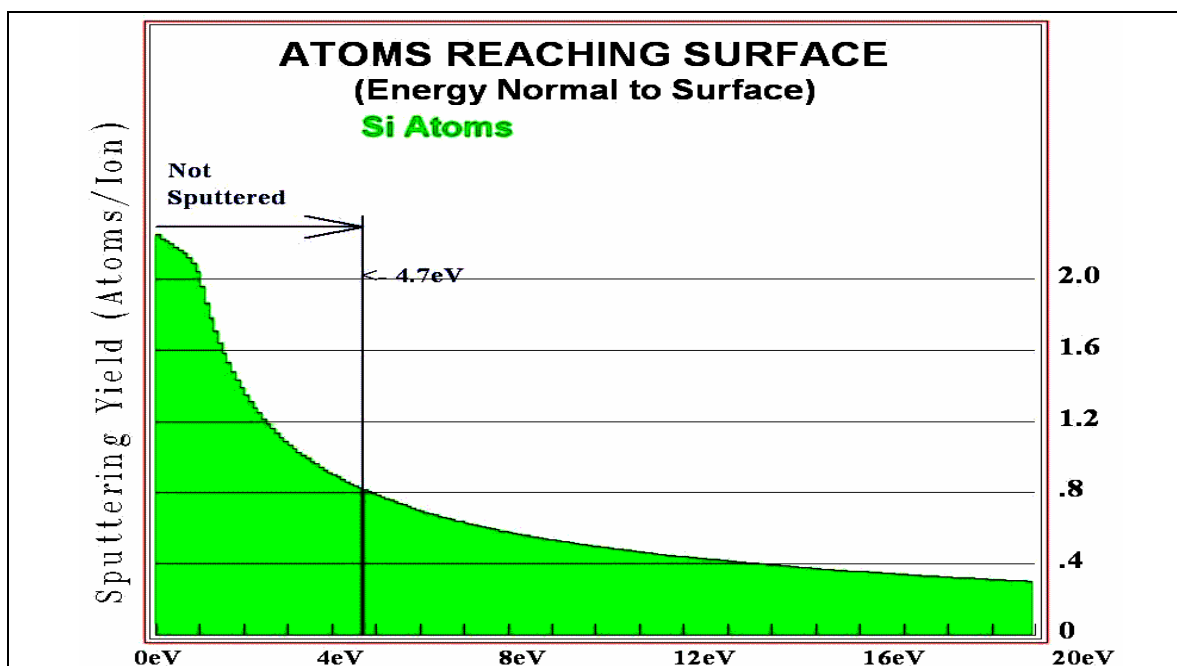
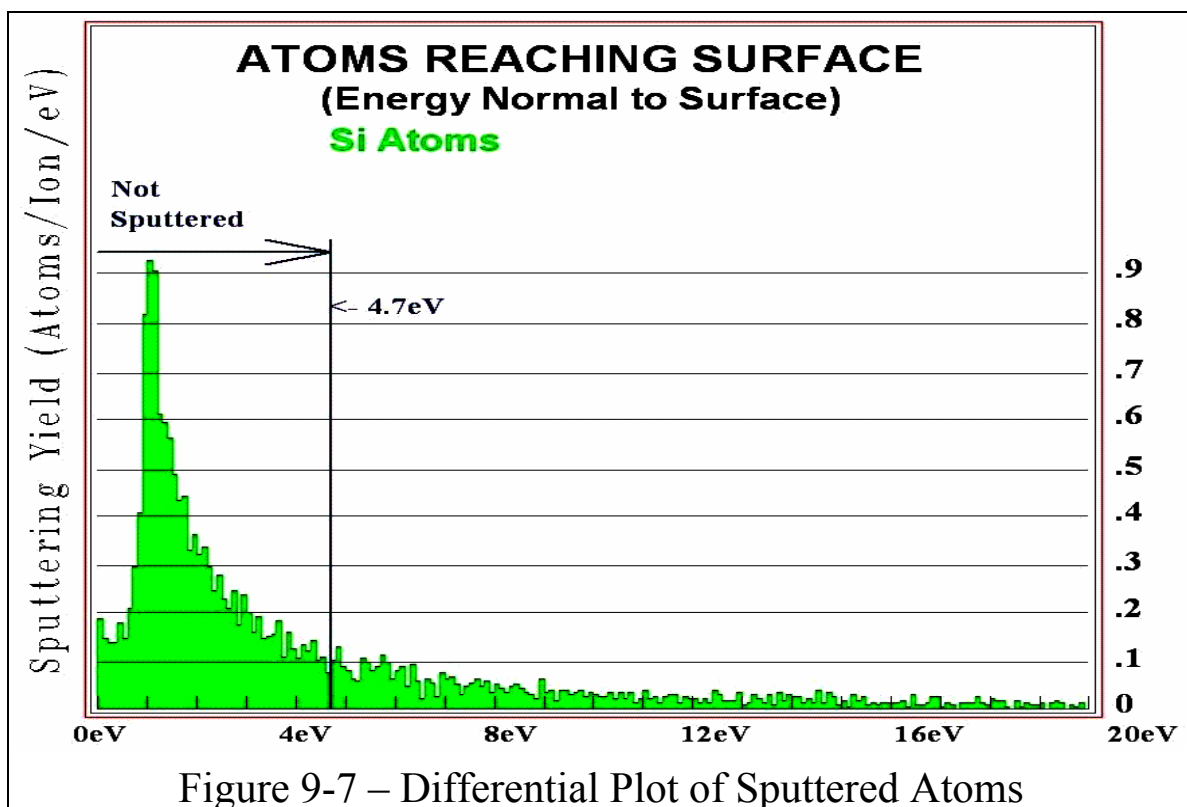


Figure 9-6 – Integral Plot of Sputtered Atoms

The plot shows the sputtering yield (atoms sputtered per incident ion) as a function of the final atom energy as it leaves the target. The SBE for W atoms was set for 3.2eV in the calculation. As shown, a great number of W atoms reached the surface without enough energy to be sputtered (the area to the left of the 3.2eV SBE). Since the SBE is not well known, this allow the user to estimate the error in using the value of 3.2 eV.

The sputtering plots can show either an Integral plot (Figure 9-6) or a Differential plot (Figure 9-7) of sputtered atom yield vs. energy. The surface binding energy for the first atom in the first layer is also indicated as a guide. The Integral plot is useful to estimate how many atoms reach the surface and do not have enough energy to leave it. The Differential plot gives an indication of how rapidly the sputtering yield will change with small changes of the SBE.



Also available is the datafile, `../SRIM Outputs/SPUTTER.txt`. The first lines of SPUTTER.TXT contain explanations of the table as well as details of the calculation, quite similar to those shown in Table 9-2 and Table 9-3. In addition, it contains the input values for the three target lattice energies, the Surface Binding Energy (SBE), the Displacement Energy (DE) and the Lattice Binding Energy (LBE), see Table 9-11.

Table 9-11 - SPUTTER.txt (Header File)

TRIM Calc.= B(200 keV) ==> Tungsten+SiO@2+Silicon(7000 A)		
Ion Data: Name,	Mass,	Energy (keV)
B	11.	200.
Displacement Energy of W = 21.0 eV		
Latt.Binding Energy of W = 2.1 eV		
SurfaceBind. Energy of W = 3.2 eV		
Displacement Energy of Si = 22.0 eV		
Latt.Binding Energy of Si = 2.2 eV		
SurfaceBind. Energy of Si = 3.2 eV		
Displacement Energy of O = 23.0 eV		
Latt.Binding Energy of O = 2.3 eV		
SurfaceBind. Energy of O = 3.3 eV		
=====		

The bottom part of the *../SRIM Outputs/SPUTTER.txt* datafile is shown in Table 9-12. The format is the same as seen for the BACKSCAT.txt and the TRANSMIT.txt files, only the leading character at the left is an “S” instead of a “B” or a “T”. Note that ion numbers 1-3 sputter no atoms, and then #4 is responsible for nine sputtered target atoms. Then ion #6 sputters one atom, and the next 14 ions sputter none. There is additional sputtering with ions #21 and #60. Often there will be no sputtering, and then one ion is scattered with a near-surface trajectory and sputters a group of surface atoms.

Table 9-12 - SPUTTER.txt (Data File)

SPUTTERING CALCULATION									
===== CALCULATION DATA =====									
Ion Data: Name, Mass, Energy (keV)									
B 11. 200.									
Displacement Energy of W = 21.00000 eV									
Latt.Binding Energy of W = 2.10000 eV									
SurfaceBind. Energy of W = 3.10000 eV									
Displacement Energy of Si = 22.00000 eV									
Latt.Binding Energy of Si = 2.20000 eV									
SurfaceBind. Energy of Si = 3.20000 eV									
Displacement Energy of O = 23.00000 eV									
Latt.Binding Energy of O = 2.30000 eV									
SurfaceBind. Energy of O = 3.30000 eV									
=====									
=This file tabulates the kinetics of ions or atoms leaving the target. =									
=Column #1: S= Sputtered Atom, B= Backscattered Ion, T= Transmitted Ion.=									
=Col.#2:Ion Number, Col.#3:Z of atom leaving, Col.#4:Atom energy (eV). =									
=Col.#5-7:Last location: X=Depth into target, Y,Z= Transverse axes. =									
=Col.#8-10: Cosines of final trajectory. =									
= *** This data file is in the same format as TRIM.DAT =									
===== TRIM Calc.= B(200 keV) ==> Tungsten+SiO@2+Silicon(7000 A) =====									
Ion	Atom	Energy	Depth	Lateral-Position			Atom Direction		
Numb	Numb	(eV)	X (A)	Y (A)	Z (A)		Cos (X)	Cos (Y)	Cos (Z)
S 4	74	.4092E+02	0000E+00	.8122E+01	.4582E+01		-.9477	.0491	.3153
S 4	74	.3783E+02	0000E+00	.5972E+01	.2946E+01		-.4821	-.8085	-.3372
S 4	74	.2115E+02	0000E+00	.3995E+01	.1648E+01		-.9992	-.0348	-.0185
S 4	74	.1014E+02	0000E+00	-.7089E+00	.7400E+01		-.8854	-.1321	.4455
S 4	74	.1236E+02	0000E+00	-.1938E+01	.7513E+01		-.6098	-.6226	.4902
S 4	74	.1372E+02	0000E+00	-.9035E+00	.4104E+01		-.9383	-.1890	.2894
S 4	74	.1586E+02	0000E+00	-.6473E+00	.1077E+01		-.4759	-.3683	-.7986
S 4	74	.3325E+02	0000E+00	.2464E+01	.5488E+00		-.9193	-.3805	-.0996
S 4	74	.1151E+02	0000E+00	.1906E+01	-.6609E+01		-.8518	.4732	-.2246
S 6	74	.1371E+02	0000E+00	.4263E+01	.1425E+01		-.8315	-.5131	.2124
S 21	74	.3334E+02	0000E+00	.7378E+00	.3956E+01		-.6313	.3118	-.7100
S 21	74	.1252E+02	0000E+00	-.1067E+01	.1999E+01		-.7440	-.6290	-.2248
S 60	74	.5663E+01	0000E+00	.6389E+03	-.8752E+03		-.8163	-.1866	.5465
---- Data Omitted from Table ----									

For correct Display of this file, use Microsoft font “Courier New” or “MS-LineDraw”. “Linedraw” is included in the SRIM software package. See the subdirectory: SRIM/Data/Linedraw.ttf

Combined Tables of Backscattering, Transmitted and Sputtering

TRIMOUT.TXT contains all the information of BACKSCAT.TXT, TRANSMIT.TXT and SPUTTER.TXT which are shown in Table 9-9 to Table 9-12. See explanations of these tables for details. TRIMOUT.TXT is generated automatically when you ask for any of the other output tables. It will only contain the data requested, e.g. if you request backscattered and sputtered data, the transmitted ion data will not be recorded.

Table 9-13 - TRIMOUT.TXT (Includes all of Table 9-9 to Table 9-11)

```

TRIMOUT.TXT: File of Transmitted / Backscattered / Sputtered Atoms
This file tabulates the kinetics of ions or atoms leaving the target.
Column #1: S= Sputtered Atom, B= Backscattered Ion, T= Transmitted Ion.
Col.#2: Ion Number, Col.#3: Z of atom leaving, Col.#4: Atom energy (eV).
Col.#5-7: Last location: X= Depth into target, Y,Z= Transverse axes.
Col.#8-10: Cosines of final trajectory.
*** This data file is in the same format as TRIM.DAT (see manual details)
TRIM Calc.= B(200 keV) ==> Tungsten+SiO2+Silicon( 7000 A)

```

Ion Numb	Atom Numb	Energy (eV)	Depth X (A)	Lateral-Position		Atom Direction			
				Y (A)	Z (A)	Cos (X)	Cos (Y)	Cos (Z)	
T	1	5	.7838E+03	7000E-03	.3092E+03	.3348E+04	.8839	.2127	-.4164
S	4	74	.4092E+02	0000E+00	.8122E+01	.4582E+01	-.9477	.0491	.3153
S	4	74	.3783E+02	0000E+00	.5972E+01	.2946E+01	-.4821	-.8085	-.3372
S	4	74	.2115E+02	0000E+00	.3995E+01	.1648E+01	-.9992	-.0348	-.0185
S	4	74	.1014E+02	0000E+00	-.7089E+00	.7400E+01	-.8854	-.1321	.4455
S	4	74	.1236E+02	0000E+00	-.1938E+01	.7513E+01	-.6098	-.6226	.4902
S	4	74	.1372E+02	0000E+00	-.9035E+00	.4104E+01	-.9383	-.1890	.2894
S	4	74	.1586E+02	0000E+00	-.6473E+00	.1077E+01	-.4759	-.3683	-.7986
S	4	74	.3325E+02	0000E+00	.2464E+01	.5488E+00	-.9193	-.3805	-.0996
S	4	74	.1151E+02	0000E+00	.1906E+01	-.6609E+01	-.8518	.4732	-.2246
S	6	74	.1371E+02	0000E+00	.4263E+01	.1425E+01	-.8315	-.5131	.2124
T	7	5	.2891E+05	7001E-03	.6063E+03	-.1998E+04	.7350	.6451	-.2084
T	10	5	.1088E+05	7002E-03	.2308E+04	.6435E+03	.9840	-.1623	-.0728
T	11	5	.9959E+04	7002E-03	.2709E+04	-.4060E+04	.7797	.3948	-.4858
B	18	5	.1562E+05	-4403E-07	.3389E+03	.1930E+04	-.7723	-.2483	.5846
S	21	74	.3334E+02	0000E+00	.7378E+00	.3956E+01	-.6313	.3118	-.7100
S	21	74	.1252E+02	0000E+00	-.1067E+01	.1999E+01	-.7440	-.6290	-.2248
B	59	5	.7361E+04	-5977E-07	-.1148E+04	-.1856E+04	-.3210	-.8717	.3700
S	60	74	.5663E+01	0000E+00	.6389E+03	-.8752E+03	-.8163	-.1866	.5465

---- Data Omitted from Table ----

For correct Display of this file, use Microsoft font "Courier New" or "MS-LineDraw". "Linedraw" is included in the SRIM software package. See the subdirectory: SRIM/Data/Linedraw.ttf

Note that every type of atom is covered here. There are 12 sputtered atoms, all of the target atom, tungsten (Z=74); there are 4 transmitted atoms, all of the incident ion, boron (Z=5); and there are 2 backscattered atoms, boron (Z=5). Since TRIM always assumes a zero-dose approximation (the incident ion does not pile up in the target), the sputtered and backscattered atoms always must be the same as the incident ion, and the sputtered atoms must always be a target atom.

Target Damage by the Ion

TRIM is often used to gain an understanding of the changes to the target under bombardment by ions. TRIM can be used for detailed examination of this target damage, but it must be interpreted with knowledge of two major TRIM limitations: (a) There is no build-up of ions or damage in the target. Every ion is calculated with the assumption of *zero dose*, i. e. the target is perfect and previous ions have no effect on subsequent ions. (b) The target temperature is 0°K, and there are no thermal effects changing the distribution of ions (thermal diffusion) or affecting the target damage (thermal annealing). Several experiments have been reported at very low temperatures (15-40°K) which validate the TRIM results, but show that thermal effects can be quite substantial. For example, for a low dose of boron ions into crystalline silicon, more than 99% of the target damage anneals at room temperature.

Full details of how TRIM calculates target damage is given in Chapter 7 and 8.

Ion's Energy Loss to the Target Electrons

The energy loss of ions to the target electrons is often called “Electronic Energy Loss” or “Ionization Losses”. These terms are synonyms. Both Plots and Datafiles are available. When ions penetrate into the target, they interact immediately with the target electrons, both single electrons and collectively. This interaction is very complicated, and TRIM uses the physics described in Chapter 3 and Chapter 7. The energy loss to electrons is collected for the TRIM Viewing Window (in 100 channels of information) and can be accessed during the TRIM calculation by selecting the **Ionization Plot** button, or the **Ionization File** button

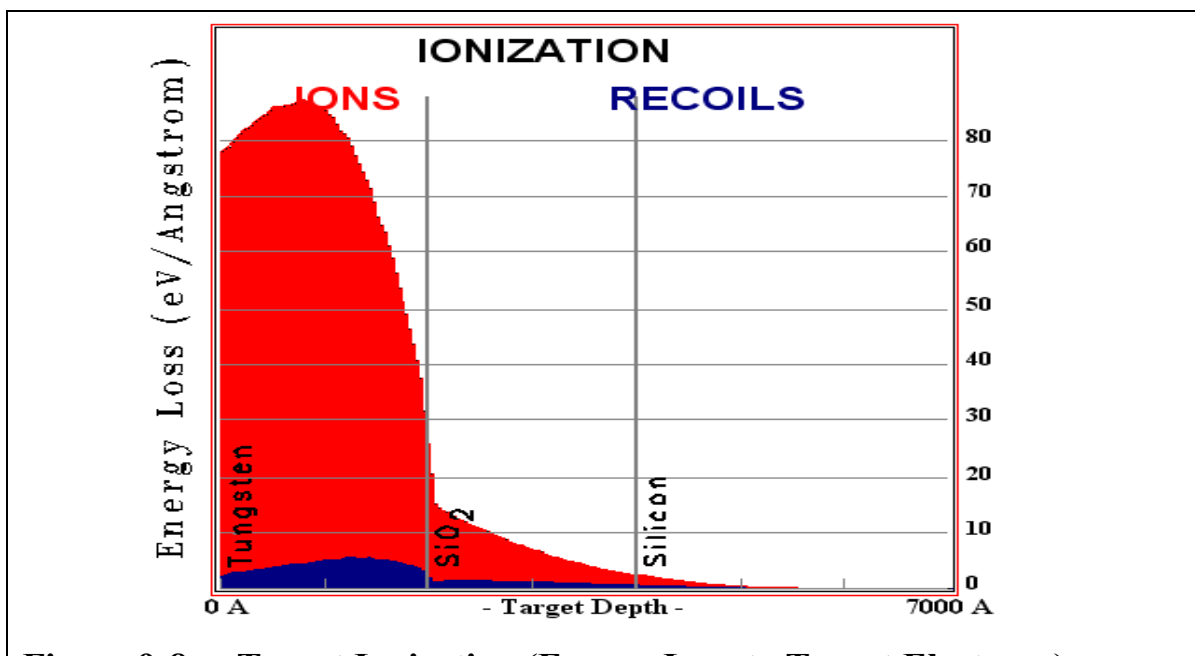


Figure 9-8 - Target Ionization (Energy Loss to Target Electrons)

The ion loses energy to the target electrons as shown in the plot in units of $\text{eV}/\text{\AA}$. This energy loss will cause target damage in insulators where the charge can build up until macroscopic damage may occur, e.g. cracking or delamination. Also shown is the electronic losses into the target caused by recoiling target atoms (dark curve). Since the recoiling atoms move relatively slowly, they have much less interaction with the faster moving target electrons

Table 9-14 - Datafile of Ionization Energy Loss in Target

<i>---- Header Information omitted from Table ----</i>		
=====		
Total Ions calculated =003859.69		
Ionization Units are >>>> eV / Angstrom / Ion <<<<		
=====		
TARGET DEPTH (Ang)	IONIZ. by IONS	IONIZ. by RECOILS
-----	-----	-----
700100.E-04	7770.18E-02	2116.60E-03
140010.E-03	7837.15E-02	2705.78E-03
210010.E-03	8014.79E-02	2966.79E-03
280010.E-03	8144.14E-02	2875.40E-03
350010.E-03	8216.98E-02	3197.69E-03
420010.E-03	8345.11E-02	3316.41E-03
490010.E-03	8418.28E-02	3501.37E-03
560010.E-03	8565.63E-02	3741.85E-03
630010.E-03	8562.24E-02	3874.91E-03
700010.E-03	8581.36E-02	4178.15E-03
<i>---- Data Omitted from Table ----</i>		

The left hand column in all tables is the depth of the bottom of each bin. The tabulated event units are usually: eV/(Å-Ion). The Header of datafile IONIZ.txt, indicates the version of TRIM used, the details of the ion and target structure, various collision parameters, and the final averages for the calculation. This header is omitted from Table 9-14.

Note that the number of ions is not an integer (here 3859.69) since the calculation was stopped in mid-flight of ion #3860. All averages are calculated including this partial ion, i.e. the Ionization/Ion = (Total Ionization) / 3859.69.

Ion's Energy Loss to the Target Phonons

When the ion collides with a target nucleus, it imparts some recoil energy to this atom. We discussed in Chapter 8 the term **Displacement Energy**, which is the minimum amount of energy that must be transferred to the target atom to knock it out of its lattice site and far enough away so it doesn't immediately fall back into this lattice hole. If the transferred energy is less than the Displacement Energy, then it is assumed that the atom returns to its lattice site and its recoil energy is transferred into target phonons. See Chapter 8 for more details.

Typical values for Displacement Energies are about 15 eV for semiconductors and 25 - 40 eV for metals. For fragile materials like polymers, a value as low as 2 - 5 eV may be more accurate.

A plot of Energy Loss to the Target Phonons is shown in Figure 9-9. The datafile, **..SRIM Outputs/PHONON.txt**, Table 9-15, stores the data of this plot as a datafile.

- The plot is created when the TRIM Calculation button "Phonons" is pressed, and then updated after each ion. The constant display of the plot slows down the calculation.

- In the plot, >90% of the phonons are produced by the recoiling atoms, while a thin line near the bottom of the plot indicates the phonons produced by the ion.

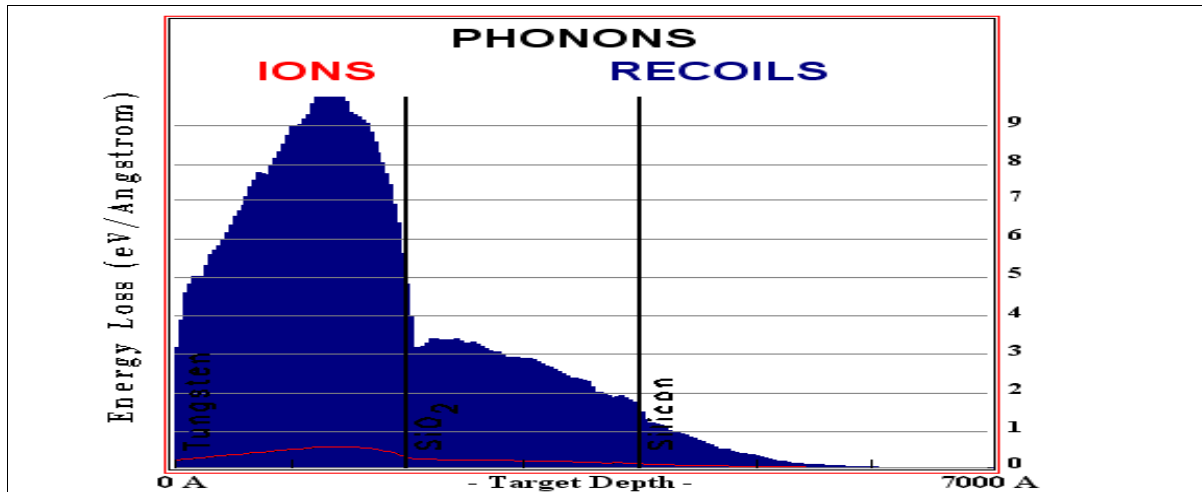


Figure 9-9 - Plot of Target Phonons

The plot shows the distribution of target phonons produced in the target.

Table 9-15 - PHONON.TXT (Energy Loss to Phonons)

---- Header Information omitted from Table ----		
Table Units are >>>> Phonons / (Angstrom - Ion) <<<<		
DEPTH (Ang.)	PHONONS by ION	PHONONS by RECOILS
700100.E-04	189790.E-06	314755.E-05
140010.E-03	209309.E-06	458183.E-05
210010.E-03	229019.E-06	500557.E-05
280010.E-03	250753.E-06	500532.E-05
---- Data Omitted from Table ----		

Energy Loss to Vacancy Production / Replacement Collisions

The plot shown in Figure 9-10 and in the datafiles, *..SRIM Outputs/VACANCY.txt* and *..SRIM Outputs/NOVAC.txt*, tabulate the energy loss to the target producing vacancies and replacement collisions. Each target atom element is shown separately. The number of vacancies depends on the Displacement Energy assigned to each target atom. A **Displacement Energy** is the minimum amount of energy that must be transferred to the target atom to knock it out of its lattice site and far enough away so it doesn't immediately fall back into this lattice hole. If the transferred energy is less than the Displacement Energy, then the atom remains in its lattice site and we assume the energy is transferred into target phonons. If it is greater than the Displacement Energy, then the new recoil has this transferred energy, minus the **Binding Energy** of the atom to its lattice site

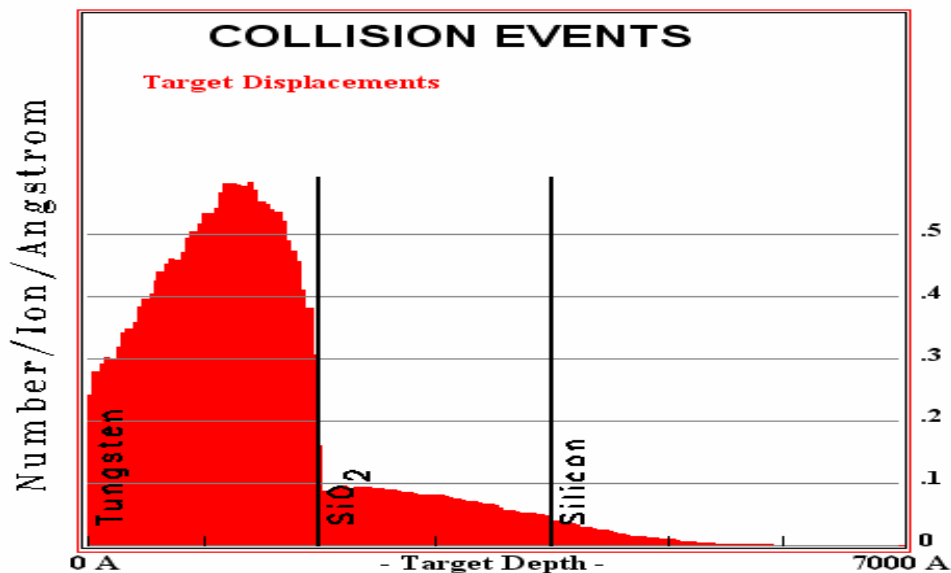


Figure 9-10 - Plot of Total Target Displacements

The plot shows the number of target atom displacements made by the incident ions. The plot includes both displacements made by the ion and by all the recoiling target atoms. These displacements will lead to either a target vacancy, or a replacements collision (see following two plots).

The above description has to be expanded for the special case of the displacement being caused not by the ion but by a recoiling target atom. If the recoiling atom knocks out a target atom, and the incoming atom does not have enough energy to go on, then it will fall into the lattice site emptied by the recoiling lattice atom. If the target atom and the recoiling target atom are the same element (which is natural since the recoiling atom probably originated in that same layer), then there is effectively no change in the target composition. For example, if an incoming recoiling W atom (110 eV) hits another W atom (with a displacement energy of 25 eV) and gives it 100 eV, the incoming ion will have only 10 eV left. This is below the displacement energy for W atoms in this layer, so it will merely replace the W atom that is knocked out. This is a **Replacement Collision**. Is this rare? No, it can be rather common, for in the target that we are using in this Chapter (see Figure 9-1), the calculation finds:

- **Total Ions calculated = 13081**
- **Average Target Displacements = 1077 /Ion**
- **Average Target Vacancies = 940 /Ion**
- **Average Target Replacement Collisions = 137 /Ion**

So the ions and recoiling atoms create 1077 displacements/ion. Of these, 940 result in vacancies, and 137 result in Replacement Collisions. So Replacement Collisions are about 13% of the total displacements. See Chapters 7 and 8 for more details.

- The plot is created in the TRIM Calculation window, when the “Damage Events” Plot button is selected. The plot is created when the button is pressed, and then updated after each ion. The display of the plot slows down the calculation.

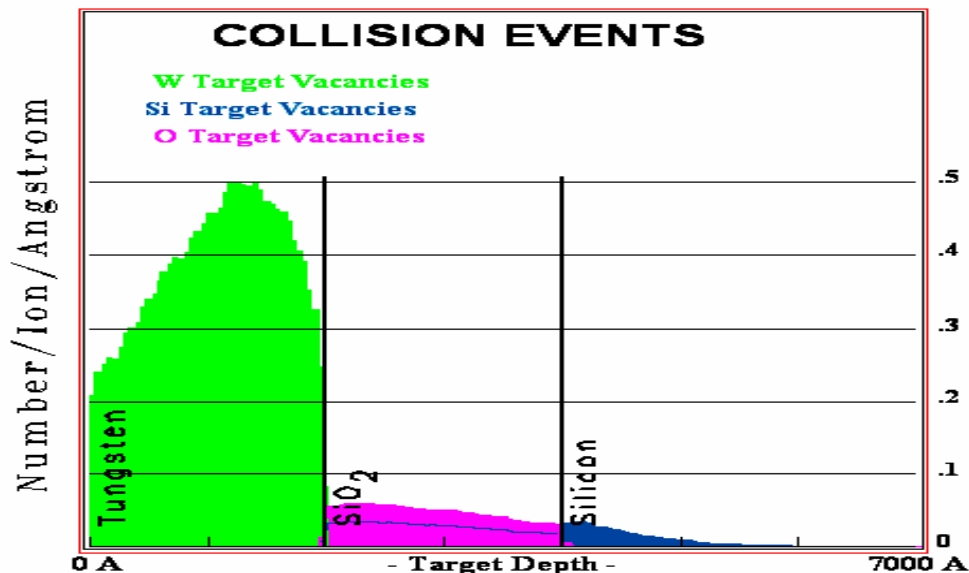


Figure 9-11 - Plot of Target Vacancies

The figure shows the plot of target vacancies, which are caused by displacements that transfer to a target atom an energy greater than that atom's Displacement Energy. Since vacancies can not migrate from the layer that contains that atom, in the upper layer are only W vacancies, and in the lower layer there are only Si vacancies. The middle layer contains two elements: Si and O, and there are two plots shown for each of types of vacancies (the plot of oxygen vacancies is a thin line).

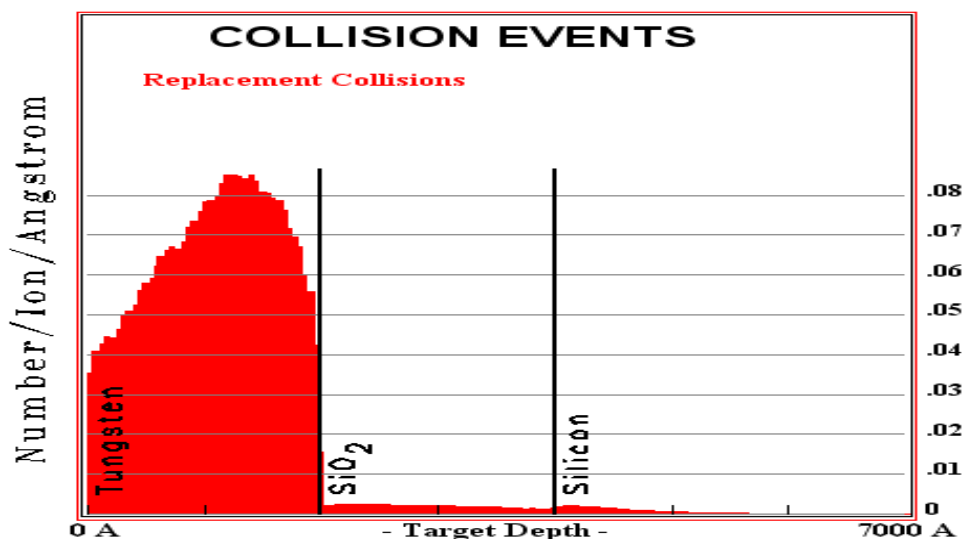


Figure 9-12 – Target Replacement Collisions

The figure shows the Replacement Collisions of the target. This is the special case where the target atom displacement is caused by a target atom of the same element, and after the collision takes place, the incoming atom does not have enough energy to leave the lattice site. Hence, it replaces the atom that it knocked out, and since it is the same elemental type, there is no change or damage to the target from this collision. Similar data for the other two layers shows a much smaller number of events in the SiO₂ and Si layers, and the datafile table has to be consulted for values.

Table 9-16 - ../SRIM Outputs/VACANCY.txt (Vacancy Production)

Ion and Target VACANCY production				
See file : SRIM Outputs\TDATA.txt for calculation data				
Ion = B Energy = 200 keV				
=====				
Total Ions calculated =13081.00				
Total Target Vacancies = 940 /Ion				
Total Target Displacements = 1077 /Ion				
Total Target Replacement Collisions = 137 /Ion				
!! NOTE : 2nd Column below is number of Primary Knock-Ons !!				
(PKO are number of Target Atoms Recoiling from the Ion.)				
=====				
Table Units are >>>> Vacancies / (Angstrom - Ion) <<<<				
=====				
DEPTH (Ang.)	B Knock-Ons	W Vacancies	Si Vacancies	O Vacancies
-----	-----	-----	-----	-----
700100.E-04	1198.08E-05	1744.28E-04	0000.00E+00	0000.00E+00
140010.E-03	1580.77E-05	2385.35E-04	0000.00E+00	0000.00E+00
210010.E-03	1714.74E-05	2599.64E-04	0000.00E+00	0000.00E+00
280010.E-03	1882.77E-05	2568.85E-04	0000.00E+00	0000.00E+00
350010.E-03	2068.05E-05	2860.98E-04	0000.00E+00	0000.00E+00
420010.E-03	2234.34E-05	2975.10E-04	0000.00E+00	0000.00E+00

The 2nd column of the datafile VACANCY.txt, Table 9-16, “B Knock-Ons” refer to vacancies directly caused by the incoming boron ion. All the other columns include both ion and recoil cascade induced vacancies.

Replacement collisions are a special type of collision in which the moving atom collides with an identical target atom, transfers an amount of energy greater than that atom's displacement energy, and does not have enough energy to move on out of the lattice site. Hence the original moving atom replaces the target atom, the target atom moves on, and since the two atoms are the same atomic species, there is no final damage. The two atoms exchange places, but since they are the same species there is no detectable change. See Chapters 7 and 8 for more details. Table 9-17 shows the Replacement Collisions which are stored in datafile: NOVAC.txt.

Table 9-17 - NOVAC.txt (Replacement Collisions)

<u>Replacement Collisions</u>	
<i>--- Header Data Omitted ---</i>	
===== TARGET MATERIAL =====	
<u>Layer 1 : Tungsten</u>	
Layer Width = 2.E+03 AAA ;	
Layer # 1- Density = 6.351E22 atoms/cm3 = 19.3 g/cm3	
Layer # 1- W = 100 Atomic Percent = 100 Mass Percent	
<u>Layer 2 : SiO@2</u>	
Layer Width = 2.E+03 AAA ;	
Layer # 2- Density = 7.015E22 atoms/cm3 = 2.33 g/cm3	
Layer # 2- Si = 33.3 Atomic Percent = 46.6 Mass Percent	
Layer # 2- O = 66.6 Atomic Percent = 53.3 Mass Percent	
<u>Layer 3 : Silicon</u>	
Layer Width = 3.E+03 AAA ;	
Layer # 3- Density = 4.989E22 atoms/cm3 = 2.32 g/cm3	
Layer # 3- Si = 100 Atomic Percent = 100 Mass Percent	
=====	
Total Ions calculated =13081.00	
Total Target Vacancies = 940 /Ion	
Total Target Displacements = 1077 /Ion	
Total Target Replacement Collisions = 137 /Ion	
=====	
Table Units are >>>> Number / (Angstrom _ Ion) <<<<	
=====	
DEPTH (A)	Number
-----	-----
7001000.E-05	0000.029330
1400100.E-04	0000.040761
2100100.E-04	0000.044445
2800100.E-04	0000.043975
3500100.E-04	0000.048435
4200100.E-04	0000.050544
4900100.E-04	0000.053586
5600100.E-04	0000.057753
<i>--- Data Omitted ---</i>	

Energy Loss from Ions – Energy Loss Absorbed by Target Atoms

There are two plots available which can be used to summarize the ion's energy that goes into recoil cascades. They are generated in the TRIM Calculation window by selecting the Plot called "*Energy to Recoils*". This generates the two plots shown below.

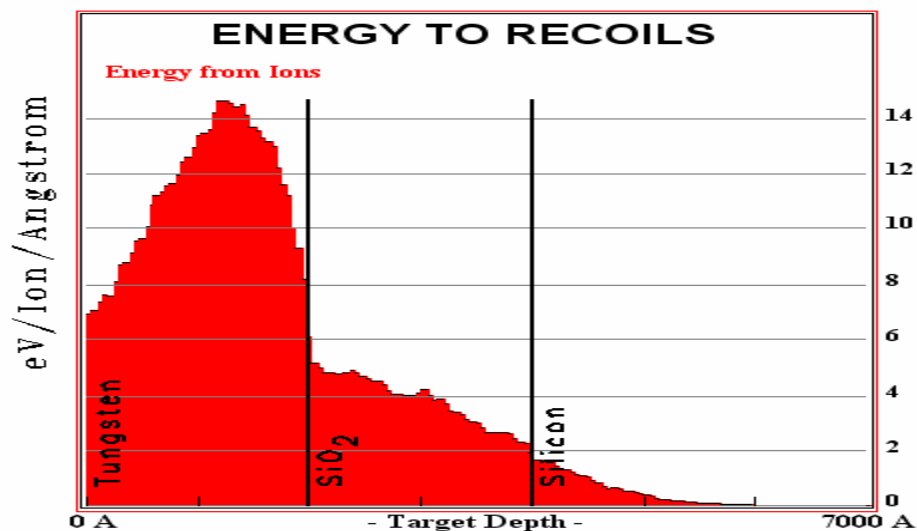


Figure 9-13 - Plot of the Energy Transferred from the Ion to Recoil Atoms

This plot shows the energy transferred from the Ion to recoils. The layer of tungsten atoms absorbs more recoil energy than the other two layers combined.

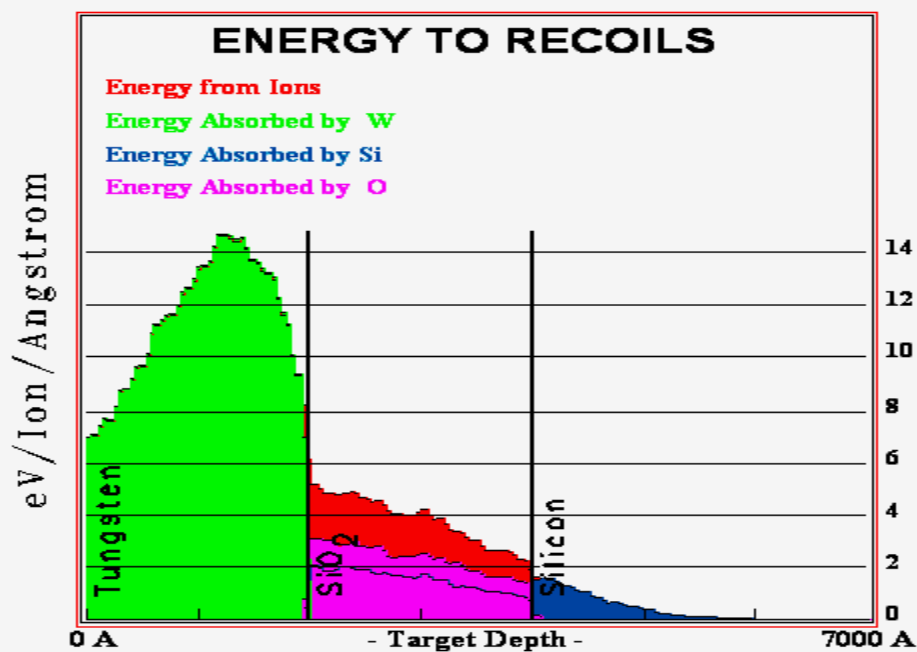


Figure 9-14 - Plot of the Energy Absorbed by the Various Target Atoms

This plot shows the amount of energy absorbed by the W, Si and O atoms of the target. It is identical to Figure 9-13 except for the middle compound layer, SiO₂. The energy in this layer is separated into that absorbed by the Si atoms and that for the O atoms (lower two lines) which add up to the energy deposited by the ions (upper curve). This plot is color-coded when viewed in SRIM and is much easier to understand.

Details of the Ion-Atom Collision Kinetics

Physics of Recoil Cascades

The following comments come from the discussions of Target Damage in Chapters 7 and 8.

The easiest way to understand the TRIM cascades is to start TRIM and select various DEMO calculations. During the calculation, play with the various plots and files, to see what they do. Each plot and file has a *Help* file associated with it, to explain its details.

Following this, you may create a more detailed understanding of cascades by selecting one of the DEMO calculations and then checking the box called "*Collision Details*", which will store every ion/atom collision in a file called "*..SRIM Outputs/COLLISON.txt*" (see Chapter on **TRIM Outputs**). Note that during the TRIM calculation, you may stop this data collection by un-checking the *Collision Detail* box in the TRIM window. This file can get quite large, so for a first experiment try it only for a few minutes of calculation time. Then stop TRIM and edit the file ***COLLISON.txt*** in the SRIM directory using any text editor. You will see tables of each ion colliding with various atoms in the target, and the detailed results of any collision cascades. Only those collisions which produce at least one displacement are tabulated, so you may not have a record of every collision.

In the file ***COLLISON.txt***, first the current ion energy and depth are given, and then the current rate of energy loss of the ion to the target electrons, i.e. the electronic stopping power, called "Se" in the table with units of eV/Angstrom. Then the target atom that is hit and starts a recoil cascade is identified, along with its recoil energy. Each cascade is then divided into displacement collisions, vacancy production, replacement collisions and interstitial atoms, as described below.

In the file, the number of Displacement collisions indicates how many target atoms were set in motion in the cascade with energies above their displacement energy (which you specified in the TRIM Setup window). The next item in the table is Target Vacancies. A vacancy is the hole left behind when a recoil atom moves from its original site. Next, the table shows Replacement collisions, which reduce the number of vacancies. If a moving atom strikes a stationary target atom and transfers more than its displacement energy to it, and the initial atom, after the collision, does not have enough energy to move onwards, and it is the same element as the atom it struck, then it just replaces that atom in the target and there is no vacancy created. Although this may sound complicated, this mechanism may reduce the total vacancies by up to 30%. The summation goes:

$$\textbf{Displacements} = \textbf{Vacancies} + \textbf{Replacement Collisions}$$

Finally, the table lists interstitial atoms. When a recoil atom stops, and is not a replacement atom, then it becomes an interstitial. These may be summed as:

$$\textbf{Vacancies} = \textbf{Interstitials} + \textbf{(Atoms which leave the target volume)}$$

If a cascade atom leaves the target volume, it is no longer followed. That is, if it leaves the target front surface or the rear surface, it is noted and then discarded. TRIM will follow atoms indefinitely as they go sideways, even though they leave your screen. But if they go through either target surface they are discarded and not counted. So vacancies occur within the target, and the final resting place of a moving recoil atom can be some distance from its vacancy. If the recoil leaves the target, clearly the sum of interstitials will be less than the number of vacancies by the

loss of that atom. Replacement collisions are not part of this equation because each replacement collision reduces the number of vacancies and the number of interstitials by one, leaving the equation in balance. Finally, an atom which comes to rest in the topmost monolayer of the target is always assumed to be a lattice atom if it originated in that layer (i.e. it is neither a replacement nor an interstitial atom).

The calculation of cascades, target displacements, replacement collisions, etc. makes certain assumptions which are defined explicitly below:

Assume an incident atom has atomic number Z_1 , and energy E . It has a collision within the target with an atom of atomic number Z_2 . After the collision, the incident ion has energy E_1 and the struck atom has energy E_2 . Previously specified for the target are energies E_d , the displacement energy, E_b , the binding energy of a lattice atom to its site, and E_f , the final energy of a moving atom, below which it is considered to be stopped.

A **displacement** occurs if $E_2 > E_d$ (the hit atom is given enough energy to leave the site). A **vacancy** occurs if both $E_1 > E_d$ and $E_2 > E_d$ (both atoms have enough energy to leave the site). Both atoms then become moving atoms of the cascade. The energy, E_2 , of atom Z_2 is reduced by E_b before it has another collision. If $E_2 < E_d$, then the struck atom does not have enough energy and it will vibrate back to its original site, releasing E_2 as **phonons**.

If $E_1 < E_d$ and $E_2 > E_d$ and $Z_1 = Z_2$, then the incoming atom will remain at the site and the collision is called a **replacement collision** with E_1 released as **phonons**. The atom in the lattice site remains the same atom by exchange. This type of collision is common in single element targets with large recoil cascades. If $E_1 < E_d$ and $E_2 > E_d$ and $Z_1 \neq Z_2$, then Z_1 becomes a stopped **interstitial** atom.

Finally, if $E_1 < E_d$ and $E_2 < E_d$, then Z_1 becomes an **interstitial** and $E_1 + E_2$ is released as **phonons**. If a target has several different elements in it, and each has a different displacement energy, then E_d will change for each atom of the cascade hitting different target atoms.

For those using the TRIM "quick" calculation of target damage, TRIM uses the Kinchin-Pease analytic solution for target damage as modified by two later authors. Typical output is shown in the Chapter 9 on **TRIM Outputs**. The following references would also help in understanding its formalism:

1. Kinchin and R. S. Pease, Rep. Prog. Phys., vol. 18, 1 (1955).
2. P. Sigmund, Rad. Eff., vol. 1, 15 (1969).
3. M. J. Norgett, M. T. Robinson and I. M. Torrens, Nucl. Eng. Design, vol. 33, 50 (1974).

COLLISON.TXT (Tabulated Detail of Collision Kinetics)

Some users need to know many more details about ions penetrating targets than is collected in the preceding plots and datafiles. For these users, it is possible to tabulate every detail of every collision between the ion and the target atoms, as well as every detail of every recoil cascade.

Details of the ion's penetration into the target can be put into a datafile, **..SRIM Outputs/COLLISON.txt**, for later examination. To get the most detailed file, in the TRIM Setup window select "Monolayer Collision Step" in the Damage menu in the upper-right corner. Then

check “*Collision Details*” in the same Setup window, at the bottom. When a sub-menu comes up and asks if details of the Recoils should also be kept, answer “*Yes*”.

This selection will overwhelm you with data. For the first **5** ions of the ion/target used in this chapter for an example (see Figure 9-1), the datafile will contain 94,000 numbers concerning 12,000 collisions. TRIM provides various filters to help you to screen this data. For example, if you are mostly interested in sampling the ion’s impact on the target, change your TRIM Setup selection from “*Monolayer Collision Step*” to “*Detailed Calculation with Full Damage Cascades*”, and the output datafile drops by 10% to 11,000 collisions. This is because TRIM now uses the Free Flight Path assumption (see Ch. 8 and 9). To further filter the data, if you care mostly about how the ion affects the target, and you can ignore the recoil cascades, then when you are in the TRIM Setup window, select “*Collision Details*” and when the sub-menu asks to store data about the recoils, answer “*No*”. This will reduce the ***COLLISON.txt*** output for the first 5 ions another 90%, down to about 1,100 collisions.

The datafile ***..SRIM Outputs/COLLISON.txt*** contains the kinetic data of all Ion-Atom collisions. The datafile is opened when the *Collision Details* button is pressed either in the TRIM Setup window, or in the TRIM Calculation window. After this selection, data is added for every subsequent collision. Three types of files may be generated, which vary in the amount of detail stored:

- **(A)** For a "Quick Damage" calculation, the damage details for each ion are summarized. No recoils are included.
- **(B)** For a "Full Recoils" calculation, the details of every ion/atom collision which leads to a displacement are itemized.
- **(C)** For a "Full Recoils" calculation, the details of every ion/atom collision and also every recoil atom/atom collision are itemized.

Special Note

These files are the most complete data files in TRIM, since they contain every significant detail of the calculation. Type “**A**” does not contain every collision, since the Free Flight Path approximation allows large jumps of the ion over many monolayers of targets without intervening collisions. (See Chapter 7, TRIM Theory, on the concept of a Free Flight Path.) This approximation may be overridden by specifying “*Use Monolayer Steps*” in the setup window for TRIM (this selection is in the upper right corner of the TRIM Setup window).

The file ***COLLISON.txt*** can increase in size very rapidly and GigaBytes of data may be generated for just a few thousand heavy ions with high energies. It is best to try a short test of ***COLLISON.txt*** to estimate the rate at which datafiles are generated.

Each of the three types of ***COLLISON.txt*** (as noted above) will be considered separately. The output file contains a notation for the various approximations used so that you can tell the conditions that generated the file.

COLLISON.txt - Type "A"– Ions and Quick Estimate of Damage

This variation on ***COLLISON.txt*** will be called type “**A**”. This ***COLLISON.txt*** datafile will contain information on every ion/target collision which results in a recoil cascade. For the "Quick Damage" calculation, TRIM uses the Kinchin-Pease approximation to predict damage based on the ion, its energy at collision, the atom hit and the target matrix. It allows for the very rapid calculation of

damage, but may be in error by up to a factor of two.

This approximation can be chosen in the TRIM Setup window, or in the TRIM Calculation window. When the **Collision Details** button is chosen in either window, a sub-menu asks whether a new file should be generated, or to add onto an existing file. Note that you must separately choose “*Ion Distribution with Quick Calculation of Damage*” (upper right corner in TRIM Setup window) in order to complete the selection of a type **A** datafile.

Table 9-18 - COLLISON.TXT (with Kinchin-Pease Damage)

--- Datafile Header Deleted ---								
Only Ion Collisions which produce Displacements are tabulated. Sums and Averages are Incomplete if Recoil Cascades Leave Target Target DISplacements = VACancies + REPLACEMENT Collisions. Target VACancies = INTERstitials + Sputtered + Transmitted Atoms Recoil Atoms which end at the surface, are not counted								
Ion Numb	Energy (keV)	Depth (Å)	Lateral Distance (Å)		Se (eV/Å)	Atom Hit	Recoil Energy (eV)	Target DISP.
			Y Axis	Z Axis				
001	19.44E+01	6556.E-03	-5879.E-04	7829.E-04	070.9	W	2692.E-03	001.000
001	18.79E+01	1108.E-02	-3462.E-03	2453.E-03	069.7	W	1391.E-02	002.372
001	18.30E+01	1983.E-02	-1796.E-02	-1620.E-03	068.9	W	9326.E-03	001.601
001	16.93E+01	3714.E-02	-3236.E-02	-5096.E-03	066.4	W	1346.E-02	002.297
001	16.46E+01	4553.E-02	-4331.E-02	1341.E-04	065.6	W	3279.E-03	001.000
001	16.46E+01	4972.E-02	-4685.E-02	5893.E-04	065.5	W	3610.E-02	006.046
001	15.87E+01	5387.E-02	-4707.E-02	-6262.E-03	064.5	W	3775.E-03	001.000
001	15.04E+01	7401.E-02	-6075.E-02	-4969.E-02	062.9	W	3549.E-02	005.947
001	13.69E+01	8856.E-02	-7700.E-02	-1139.E-01	060.4	W	4198.E-03	001.000

The datafile shown in Table 9-18 starts when ion #001 enters the target and has its first collision at a depth of 6.56Å when it has an energy of 194.4 keV. (Because of the Free Flight Path, there is not a collision in every target monolayer.) The Lateral Distance column shows a slight displacement from the original ion axis. The ion hits a W atom, and gives up 2.69 eV to this atom. It creates 1.0 target displacements. Note that other harder collisions in the table generate fractional displacements since the displacements are calculated using the Kinchen-Pease approximation. If you wish to make the ion interact with every monolayer of the target, then in the TRIM Setup window specify “*Use Monolayer Collision Steps*”.

Unlike the detailed damage and recoil data shown in the *COLLISON.txt* files type **B** and **C**, described below, for the Kinchin-Pease approximation there is only a single estimate of the target displacements produced. This calculation is made with the same random numbers as that of the more detailed tables of the “*Full Recoils*” calculation, so there is a direct correspondence in collisions. In general, Kinchen-Pease estimates more displacements than TRIM with full recoil cascades.

COLLISON.txt - Type “**B**”– Ions and Recoil Atoms (no cascade data)

This variation on *COLLISON.txt* will be called type “**B**”. This version of *COLLISON.txt* shows only those collisions which result in a recoiling target atom, i. e. only those collisions in which the ion transfers to the target atom an energy greater than its displacement energy (which was entered in the setup program). Additionally, this datafile contains additional information as noted below:

This approximation can be chosen in the TRIM Setup window, or in the TRIM Calculation window. When the **Collision Details** button is chosen in either window, a sub-menu asks whether a new file should include data for Recoil. Select “No” to generate this type **B** datafile. Note that you must separately choose “Detailed Calculation with Full Damage Cascades” or “Use Monolayer Collision Steps” (menu in the upper right corner in TRIM Setup window) in order to complete the selection of a type **B** datafile.

In the file below, *Se (eV/Å)* is the electronic stopping power of the ion in the target at its current energy. This energy is modified by including a straggling component (random variation) in the calculation, so that the actual ion electronic energy loss between specific collisions can not be directly obtained from this number. Because of mathematically required statistical fluctuations, the ion energy may actually increase between collisions (this sounds crazy, but it really is true).

Target **Displacements, Vacancies, Replacement Collisions, and Interstitial Atoms** were described previously in this chapter in the section **Physics of Recoil Cascades**. They are also described in Chapter 7 - **TRIM Theory**. These types of damage constitute the changes introduced into the target by each collision. Since data on recoils was not requested for a type **B** datafile, the final results of each collision cascade are given in four columns of target damage (number of displacements, vacancies, replacement collisions and interstitial atoms).

Table 9-19 - COLLISON.txt (Recoil Atoms without cascade data)

===== COLLISION HISTORY											
NOTES: Only Ion Collisions which produce Displacements are tabulated.											
Atom Sums and Averages are Incomplete if Recoil Cascades Leave Target.											
Target DISplacements = VACancies + REPLACEMENT Collisions.											
Target VACancies = INTERstitials + Sputtered + Transmitted Atoms.											
Recoil Atoms which end at the surface, are not counted (see manual).											
Ion Numb	Energy (keV)	Depth (Å)	Lateral Distance (Å)		Se (eV/Å)	Atom Hit	Recoil Egy (eV)	Tgt DISP.	Tgt VAC.	Tgt REPL	Tgt INTER
			Y Axis	Z Axis							
001	19.44E+01	65564.E-03	-5879.E-04	7829.E-04	0070.90	W	26922.E-03	002	001	001	002
001	18.44E+01	15224.E-02	-7317.E-03	3660.E-03	0069.15	W	75609.E-03	006	005	001	006
001	17.99E+01	31873.E-02	-2894.E-02	2599.E-02	0068.34	W	33106.E-02	011	010	001	011
001	17.19E+01	39161.E-02	-4127.E-02	2706.E-02	0066.90	W	89507.E-03	005	003	002	005
001	17.03E+01	43332.E-02	-4873.E-02	3179.E-02	0066.62	W	94263.E-03	006	006	000	006
001	15.60E+01	62681.E-02	-1008.E-01	5174.E-02	0064.01	W	92898.E-03	004	002	002	004
001	15.13E+01	71468.E-02	-1331.E-01	4748.E-02	0063.14	W	46885.E-03	003	003	000	003
001	14.63E+01	75113.E-02	-1468.E-01	4719.E-02	0062.22	W	52406.E-03	003	003	000	003

For correct Display of this file, use Microsoft font “Courier New” or “MS-LineDraw”. “Linedraw” is included in the SRIM software package. See the subdirectory: SRIM/Data/Linedraw.ttf

COLLISON.txt - Type "C"– Ions, Recoil Atoms and Cascades

This variation on *COLLISON.txt* will be called type "C". This version of *COLLISON.txt* includes all the ion/target collisions which result in a recoiling target atom, and also the history of what happens to that recoiling atom and also any atoms that recoil hits, i.e. the full details of the full recoil cascade.

Table 9-20 - COLLISON.txt (Full Recoil Cascades)

===== COLLISION HISTORY =====

NOTES: Only Ion Collisions which produce Displacements are tabulated.
Atom Sums and Averages are Incomplete if Recoil Cascades Leave Target.
Target DISplacements = VACancies + REPLACement Collisions.
Target VACancies = INTERstitials + Sputtered + Transmitted Atoms.
Recoil Atoms which end at the surface, are not counted (see manual).

=====

Ion Numb	Energy (keV)	Depth (A)	Lateral Distance (A)		Se (eV/A)	Atom Hit	Recoil Egy(eV)	Tgt DISP.	Tgt VAC.	Tgt REPLAC	Tgt INTER
			Y Axis	Z Axis							

001 9.4E+01 65564.E-03 -587.E-04 7829.E-04 0070.90 W 26922.E-03 <== New Cascade

=====

Recoil	Atom	Energy(eV)	X (A)	Y (A)	Z (A)	Vac	Repl	Ion Numb	00001=
--------	------	------------	-------	-------	-------	-----	------	----------	--------

00001 74 26922.E-03 6556.E-02 -5879.E-04 7829.E-04 1 00 <-Prime Recoil

00002 74 00000.E+00 6577.E-02 1880.E-03 1167.E-03 0 01

00003 74 22058.E-03 6577.E-02 1880.E-03 1167.E-03 1 00

=====

Summary of Above Cascade ==> 002 001 001 002

001 18.4E+01 15224.E-02 -7317.E-03 3660.E-03 69.15 W 75609.E-03

== New Cascade

=====

Recoil	Atom	Energy(eV)	X (A)	Y (A)	Z (A)	Vac	Repl	Ion Numb	00001=
--------	------	------------	-------	-------	-------	-----	------	----------	--------

00001 74 75609.E-03 1522.E-01 -7317.E-03 3660.E-03 1 00 <-Prime Recoil

00002 74 33842.E-03 1517.E-01 -6850.E-03 -1038.E-03 1 00

00003 74 27773.E-03 1504.E-01 -7967.E-03 -2840.E-03 1 00

00004 74 24541.E-03 1483.E-01 -7860.E-03 -1394.E-03 1 00

00005 74 26789.E-03 1527.E-01 -6710.E-03 1267.E-03 1 00

00006 74 00000.E+00 1530.E-01 -8912.E-03 2419.E-03 0 01

00007 74 23177.E-03 1530.E-01 -8912.E-03 2419.E-03 1 00

=====

Summary of Above Cascade ==> 006 005 001 006

001 17.99E+01 31873.E-02 -2894.E-02 2599.E-02 0068.34 W 33106.E-02

== New Cascade

=====

Recoil	Atom	Energy(eV)	X (A)	Y (A)	Z (A)	Vac	Repl	Ion Numb	00001=
--------	------	------------	-------	-------	-------	-----	------	----------	--------

00001 74 33106.E-02 3187.E-01 -2894.E-02 2599.E-02 1 00 <-Prime Recoil

00002 74 41182.E-03 3156.E-01 -2969.E-02 3458.E-02 1 00

00003 74 24907.E-03 3168.E-01 -3053.E-02 3254.E-02 1 00

00004 74 21368.E-03 3166.E-01 -3245.E-02 3414.E-02 1 00

00005 74 51224.E-03 3171.E-01 -3061.E-02 3005.E-02 1 00

00006 74 14846.E-02 3187.E-01 -3019.E-02 2816.E-02 1 00

00007 74 98698.E-03 3187.E-01 -3254.E-02 2904.E-02 1 00

00008 74 73706.E-03 3187.E-01 -3505.E-02 2896.E-02 1 00

00009 74 67029.E-03 3187.E-01 -3289.E-02 3024.E-02 1 00

00010 74 29954.E-03 3186.E-01 -3150.E-02 3232.E-02 1 00

00011 74 00000.E+00 3185.E-01 -3174.E-02 2983.E-02 0 01

00012 74 22731.E-03 3185.E-01 -3174.E-02 2983.E-02 1 00

=====

Summary of Above Cascade ==> 011 010 001 011

001 17.19E+01 39161.E-02 -4127.E-02 2706.E-02 0066.90 W 89507.E-03

== New Cascade

----- Data Omitted -----

For correct Display of this file, use Microsoft font “Courier New” or “MS-LineDraw”. “Linedraw” is included in the SRIM software package. See the subdirectory: SRIM/Data/Linedraw.ttf

Table 9-20 is quite complicated since it contains all the kinetic information about every ion collision, as well as the data for every recoil collision. One must be careful of using this type of file because strong recoil cascades may involve 10,000+ sub-collisions which can rapidly make the file unmanageable.

This approximation can be chosen in the TRIM Setup window, or in the TRIM Calculation window. When the **Collision Details** button is chosen in either window, a sub-menu asks whether a new file should include data for Recoil. Select “Yes” to generate this type **C** datafile. Note that you must separately choose “Detailed Calculation with Full Damage Cascades” or “Use Monolayer Collision Steps” (upper right corner in TRIM Setup window) in order to complete the selection of a type **C** datafile.

See the comments for *COLLISON.txt*, type “**B**”, for details about most of this table. The additional information is for the recoil cascades.

Analysis of Table 9-20 - COLLISON.txt (Full Recoil Cascades)

The calculation shown did not demand monolayer collisions (where the ion impacts a target atom every monolayer). Hence, the Free Flight Path approximation (see Ch. 8 and 9) allowed the ion to jump 66Å into the target for its first collision which transfers 27eV, and this causes the recoil to start a 3 atom cascade. This cascade is shown in detail in the box between this collision and next ion collision. The first line in this box shows the primary recoil (identified with “<- **Prime Recoil**”) and then the succeeding recoils. If some of these secondary recoils cause further recoils, the box gets complicated. But each recoil is followed until it reaches zero energy, and then the last recoil it caused is tracked, etc. until the first recoil caused by the prime recoil is tracked. For a monoatomic target, Displacements = Vacancies + Replacements = Replacements + Interstitials. For more details, see brief explanation called *Physics of Recoil Cascades* which was copied from Chapter 7. More details are in Chapters 7 and 8. Note that the “Final Summary” of each cascade showing the target damage is identical in type “**B**” and type “**C**” tables.

Special Commands for a TRIM Calculation

Changing TRIM Parameters during the Calculation

Note that TRIM can be stopped during the calculation, and basic parameters may be changed. This allows the user to focus the calculation on a specific problem without having to start over. To change TRIM during a calculation, click on the button **Pause TRIM** at the top of the TRIM Calculation window. Then press **Change TRIM**. All the parameters which can be changed will have a yellow background, and it includes almost all Setup parameters. Make changes in the parameters, or in the colors used for the plots (clicking on the colors in the Target Data window will bring up a color-chart to use). When you are done, press **End Edit** and then **Continue**. You will be asked if you wish to add the next calculation to the previous results, or restart TRIM.. This procedure allows the user to modify a TRIM calculation simply, or include ions of different energies or incident angles (for example) into one plot. See Chapter 8 for more details.

Changing TRIM Plots and Colors (TRIM.cfg)

All of the TRIM plots and colors are set using the datafile: `../Data/TRIM.cfg`, see Table 9-21. Typical default settings are shown in this Table. If you change TRIM colors, e.g. using the color tables available in the TRIM Calculation window, then when you save TRIM these changes become the default values.

Table 9-21 -Datafile `../Data/TRIM.cfg` (TRIM Plots and Colors)

```
[Ion Colors - MOVE, STOP]
255      0
[12 Recoil Colors - MOVE, STOP]
1        6487906   837122
2        15982183  16417654
3        16744703   12519886
4        16777088   13814035
5        13159423   9673727
6        16760769   16711680
7        8421376    65280
8        6422724    12615935
9        8388736    16716287
10       4755857    8700353
11       9408399    12566463
12       255       0
[Distribution Plot Labels - SIZE, COLOR]
6        8388608
[4 Distribution Plot Colors]
255      8388608   65280   16776960
[Plot Background, Outer Box, Axes, Layer Lines, Layer Names]
16777215 255 0 0 0
Maximum number of secondary recoils (default=20000)
20000
Note: 100k recoils requires 2MB of memory, 1M recoils requires 35MB.
```

The colors are identified by standard PC color codes, which are too complicated to review here. For example, the Ion Color is RED (#255) when it has a collision, and BLACK (#000) for the point where it stops. The target recoil atoms are identified by numbers 1-12 in the next section of Table 9-21. However, it is easiest to start a TRIM calculation, and then click on the button ***Pause TRIM*** at the top of the TRIM Calculation window. Then press ***Change TRIM***. Expand the sub-window called **Target Data** and you will see bars of color for each of the target elements. Click on any one, and you can select a new color from a color grid. Change as many colors as you want, and see how they look by pressing ***Continue*** and opening a plot. When you finally stop the TRIM calculation and save it, these new colors will be stored as the default recoil atom colors.

Making TRIM Animated Plots

Normally TRIM waits until the end of each ion's path before plotting the details of this trajectory on the TRIM plots. However, it is possible to plot each collision as it occurs. In the TRIM Calculation window, in the **ION** sub-window, there is a box called **SHOW LIVE DATA**. You may press this at any time, and a new window will pop up, and show the ion's position (x, y, z coordinates) its energy, and the energy transferred to any cascade that it makes. The data moves

rather fast, but a quick finger can hit **Pause** to stop the ion at any instant to see where it is and what size cascade it has made. This display slows down the calculation.

To end this display, click on **END LIVE DATA**, and after the current ion completes its path, the sub-window will close and the calculation will resume normally.

TRIM “Help, FAQ and Scientific Explanations”

At the top of the TRIM Calculation window is a tab called **Help, FAQ and Scientific Explanations**. Many of the concepts of TRIM are in this file, and it is useful to read explanations while the TRIM calculation proceeds. It also has **Help** files for common errors that might occur.

Among the available topics are:

- **The Scientific Background of TRIM**
 - **Physics of Recoil Cascades**
 - **Physics of Sputtering**
 - **The Stopping of Ions in Compounds**
 - **Stopping Powers for Ions in Gases**
- **Special Applications of TRIM**
 - **3-D Plots of Electronic Energy Loss**
 - **Isotopically Enriched Targets**
 - **Ion Energy Reducers (Energy Degraders)**
 - **Adding Together Sequential TRIM Calculations**
 - **High Resolution Collision Data**
 - **Ion Mixing Experiments**
- **TRIM FAQ and Solutions**
 - **Printing Problems**
 - **High Resolution Plots**
 - **Statistics of Range Distributions**
 - **Peaks and Dips at Layer Edges**
 - **Auto-TRIM (Running TRIM in Batch Mode)**
- **Identification of TRIM Programs and Software**

