8 - TRIM – SETUP AND INPUT [*]

TRANSPORT OF IONS IN MATTER

TRIM is Monte Carlo computer program that calculates the interactions of energetic ions with amorphous targets. The specific science and mathematics behind the program were summarized in Chapter 7. This chapter reviews the use of TRIM to evaluate many different kinds of calculations. Most of this chapter may also be found in the Help menus included in the TRIM program. See also Chapter 9, TRIM Output Files, for an explanation of the various TRIM output plots and files.

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[*] **Note: This text is from Chapter 8 of the SRIM textbook (2008):**

"SRIM – The Stopping and Range of Ions in Matter"

Introduction

TRIM is a group of programs which calculate the stopping and range of ions (10 eV - 2 GeV/amu) into matter using a quantum mechanical treatment of ion-atom collisions (this manual refers to the moving atom as an *"ion"*, and all target atoms as *"atoms"*). This calculation is made very efficient by the use of statistical algorithms which allow the ion to make jumps between calculated collisions and then averaging the collision results over the intervening gap. During the collisions, the ion and atom have a screened Coulomb collision, including exchange and correlation interactions between the overlapping electron shells. The ion has long range interactions creating electron excitations and plasmons within the target. These are described by including a description of the target's collective electronic structure and interatomic bond structure when the calculation is setup (tables of nominal values are supplied). The charge state of the ion within the target is described using the concept of effective charge, which includes a velocity dependent charge state and long range screening due to the collective electron sea of the target. A full description of the calculation is found in Chapter 7.

TRIM will accept complex targets made of compound materials with up to eight layers, each of different materials. It will calculate both the final 3D distribution of the ions and also all kinetic phenomena associated with the ion's energy loss: target damage, sputtering, ionization, and phonon production. All target atom cascades in the target can be followed in detail. The programs are made so they can be interrupted at any time, and then resumed later. Plots of the calculation may be saved, and displayed when needed.

TRIM Setup Window

TRIM is contained in the programs called SRIM (The Stopping and Range of Ions in Matter). It can be accessed from its Title page by pressing the button marked TRIM. The easiest way to understand TRIM is to try one of the demonstration calculations. These have been selected to illustrate many of the variations available in TRIM. In the Setup Window, Figure 8-1, see button: **TRIM Demo**.

The TRIM Tutorials are especially recommended to understand how to setup TRIM (see Chapter 11 and also www.SRIM.org). These tutorials will explain in detail each of the required TRIM inputs.

Figure 8-1 - TRIM Setup Window

The **TRIM Setup Window** is used to input the data on the ion, target, and the type of TRIM calculation that is wanted. Almost all inputs have online explanations. To become familiar with the various types of calculations, it is easiest to use the **TRIM Demo** menu to see how various applications look in the Setup Window. Each of the entries above is discussed in this chapter.

Types of TRIM Calculation (Menu in upper-right corner)

- **Ion Distribution and Quick Calculation of Damage** - This option should be used if you don't care about details of target damage or sputtering. The damage calculated with this option will be the quick statistical estimates based on the Kinchin-Pease formalism (see section *Physics of Recoil Cascades* for details about target damage). The following data will be calculated correctly: Final distribution of ions in the target, Ionization energy loss by the ion into the target, Energy transferred to recoil atoms, Backscattered Ions and Transmitted Ions. You will get identical ion range results as when you use the *Full Damage Cascade* option below, since the random number generator for the ions is separate from that used for the recoils. This is useful to compare calculations.

- **Detailed Calculation with Full Damage Cascades** - This option follows every recoiling atom until its energy drops below the lowest displacement energy of any target atom. Hence all collisional damage to the target is analyzed. The one exception is for very rare massive cascades which exceed 20,000 atoms. At this point TRIM runs out of memory, and an error

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message is posted indicating that the limit of 20,000 recoiling atoms in a single cascade has been exceeded. The calculation continues after the message is posted. This error can be eliminated using the datafile: *..\Data\TRIM.cfg*. See the later section in this chapter on "*Changing Maximum Size of Recoil Cascades (TRIM.cfg)*"

- *Monolayer Collision Steps* – This calculation requires TRIM to make the ion have a collision in each monolayer of the target. This omits any use of the **Free Flight Path**, described in Chapter 7, and every collision will be calculated without any approximations. The results of using this option will ultimately give the same averaged quantities such as mean range, ionization, damage, etc., but the calculation will take far longer to execute. This type of calculation is essential for special applications such as sputtering (below) and to generate data on every possible collision in the file *COLLISON.txt* (see Chapter 9 for more details).

- *Calculation of Surface Sputtering* - This calculation requires TRIM to make the ion have a collision in each monolayer of the target, which is essential for an accurate calculation of ion sputtering. Special plots are available to aid in understanding the special physics of sputtering. They allow you to analyze the effect of small variations on the Surface Binding Energy on the sputtering yield. This parameter is at the heart of sputtering, and its value is sometimes difficult to estimate. TRIM provides a table of Heat of Sublimation values, which are the normal starting values in estimating the surface binding energy of a target (see file *../Data/ATOMDATA*). There is no significant difference in choosing this item over the previous selection above. (Details are found in the later section in this chapter called *"The Physics of Sputtering"*.)

- *Neutron / Electron / Photon Cascades* - This option is used to calculate only the damage cascades in a target. It uses as input the file **TRIM.DAT** which contains the kinetic information about atoms which start recoil cascades. The file **TRIM.DAT** is generated by some other program which calculates the energy transferred to target atoms by either neutrons, electrons or photons. Then TRIM takes this external information and calculates the damage done to the target from recoil cascades. This is explained in the special TRIM application section "*Radiation Damage from Neutrons / Electrons / Photons*". If you select this option, you will get a sub-menu which requests which kind of damage calculation you wish to make.

- *Various Ion Energy / Angle / Positions* - This option allows the calculation of TRIM with ions starting at various energies, or with varying trajectory angles to the target surface, or starting at various depths in the target. There are a wide range of applications which require the ability to vary these ion parameters, and they are discussed in the section *"Ions starting with various Energy / Angle / Position"*. Typical are calculations of ions from a diffuse plasma, or for a target with a receding surface due to rapid sputtering, or reactor radiation damage to metals. This option requires the file **TRIM.DAT** for the initial ion energy, trajectory and starting position. If you select this option, you will get a sub-menu which requests which kind of damage calculation you wish to make.

- *Special Multi-Layer Biological Targets* - TRIM allows the calculation of complex biological targets with up to eight layers using standard ICRU and ICRP target designations. This setup is special, and if you want this calculation you should read the section on *Special Setup for Multi-Layer Biological Targets*, later in this manual.

Ion Name, Mass, Energy

- Enter the ion name, e.g. O for oxygen or He for helium (TRIM ignores the case of the letters). It is usually convenient to press $\boxed{\text{PT}}$, see Figure 8-2, to obtain a Periodic Table of Elements, and just click on the element. For the ion mass, TRIM suggests the mass of the most abundant isotope (not the natural weight). These values are shown in the Periodic Table as MAI (Most Abundant Isotope). However, you may enter any mass (units = amu). For the ion energy, enter

any value (units = keV). TRIM will accept any values from 10 eV to 10 GeV/amu. One should be cautioned that TRIM does not include any nuclear reaction analysis, so that ions with energies above about 5 MeV/amu may have inelastic energy losses which are not included in its calculation.
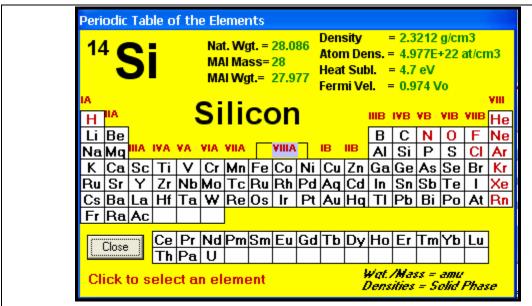

Figure 8-2 – Periodic Table of Elements

The TRIM Setup window provides the user with a Periodic Table of Elements for the ion and target atoms. An element is selected the button PT and then clicking on an element. Also provided are the default parameters for that element. MAI is the most abundant isotope, which is typically the isotope used for the ion. The Heat of Sublimation is the default value for the surface binding energy of a solid (used for sputtering) and the Fermi Velocity, V_0, is used to calculate the stopping power in that element, given in units of $V_0 \sim 1.3 \times 10^6$ m/s.

● **PROBLEM NOTE:** To setup TRIM, you have to declare in Windows that your Regional Setting is "English (United States)", which uses a period as a decimal point. This is explained in the ReadMe file in the SRIM root directory (which helps correct initial SRIM installation errors). Basically, you must do the following:

o Open "*My Computer*"
o Open "*Control Panel*"
o Open "*Regional Settings*".
o Set your Regional Settings to "English (United States)".
o You can now check that the decimal point is now a period by selecting the Tab called "*Number*". It should show a period for the "*Decimal Symbol*".
o Close the Regional Settings window.
o *It is NOT necessary to restart your computer.*
o When you complete using TRIM, you can reset your Regional Settings without restarting your computer.

• *Angle of Incidence of Ion* - This varies the angle of incidence of the ion with respect to the target surface. Normally, the ion is perpendicular to the target surface, along the X-axis at an angle defined as 0°. This angle may be changed to any angle from 0 - 89.9°. The change in ion direction is assumed to be in the XY plane.

Target Description

- **Solid or Gas Target** - TRIM treats gas targets different from solid targets. You must declare your target phase here. If your target has mixed gas and solid layers, then you need to read the later section *"Using TRIM with Mixed Gas / Solid Targets"*. Targets containing normal gases such as oxygen, in solid form such as in a quartz target, should be declared as solids. The interaction of ions with atoms in solid phase is treated differently than for those atoms in gases. See Chapter 5.

- **Target Elements** - Input the various elements which make up your target, in the same way that you input your ion, e.g. Si = silicon. The same Periodic Table of Elements is available using the button PT, see Figure 8-2. Using this table, you will see the default values used for each target element. You may enter up to twelve target elements per layer. One special application of TRIM is to follow the mixing of layers by ion beams which create cascades. If, for example, you wish to follow silicon atoms from a surface layer of SiO_2 mixing into a silicon substrate, you can specify the target element Si twice, once for the surface layer and once for the substrate. TRIM will keep the two Si atoms separate, and you will be able to distinguish one from the other in the various analytic plots.

- **Table of Compounds** - TRIM has an encyclopedia of common compounds available for simple single-layer targets. In the TRIM Setup window, by pressing Compound Dictionary these tables are accessed. In addition to the compound stoichiometries, this table provides typical densities and also bonding information. For many light compounds, especially hydrocarbons, this bonding information is later used to make significant corrections to the stopping powers. When you use this table, you will be able to skip over most of the target input steps. See Chapter 5 for special considerations when you have a compound target.

- **Layer Depths and Stoichiometry** - Once you have entered your list of target elements, you will build up your target layers (up to eight layers). Enter the first target thickness. The default units are Angstroms, however you may also used units of microns, millimeters, meters or kilometers by using the drop-down menu of units. For each layer, you will enter the amount of each element in that layer. TRIM normalizes this input, so you may use any units. For example, for a target of SiO_2 you may use any of the following: Si(1) O(2); Si(100) O(200); Si(33) O(67); etc.

- **Layer Density** - Each layer must have a density (units = g/cm^3). TRIM will guess at densities, using a mixture of elemental target densities weighted by their relative stoichiometry. However, you should be careful to check that the density is reasonable. ***The final TRIM distributions will scale with target density, so any errors in density will directly transcribe into errors in ranges, etc.***

- **Layer Name** - Each layer is described on the plots and in all the data files using the name you input here. You can use simple names such as Silicon, or SiO2, or more detailed descriptive names such as Si(33)-Ge(67).

> You can have TRIM print subscripts and superscripts for layer names on the plots by using the special commands **$** (superscript**)** and **@** (subscript). The name *SiO@2* will print on the screen as SiO_2. 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 "Fe_2O_3" for that layer name.

Damage Energies of Target Atoms

On the far right of the target data are three entries for: *Damage (eV) / Disp., Latt., Surf*. These are the values for the target atoms *Displacement Energy, Lattice Binding Energy, and Surface Binding*

Energy. .These quantities were discussed in detail in chapter 7 on TRIM Theory. TRIM provides default values for every element.

- **Displacement Energy** - This is the energy that a recoil needs to overcome the target's lattice forces and to move more than one atomic spacing away from its original site. If the recoiling atom does not move more than one lattice spacing, it is assumed that it will hop back into its original site and give up its recoil energy into phonons. Typical values are about 15 eV for semiconductors and 25 eV for metals. For fragile materials like polymers, a value as low as 2 - 5 eV may be more accurate. For users who understand the physics of displacements, individual energies may be input for each of the different target atoms. For targets with several layers containing the same element, for example SiO_2 on Si, you may use different displacement energies for Si atoms in the two layers.

- **Surface Binding Energy** - If you are interested in sputtering, then this parameter is key to the sputtering yield (number of target atoms leaving the target surface). This is the energy that target atoms must overcome to leave the surface of the target (units = eV). Note that this is not the traditional chemical binding energy for surface atoms, for it includes all surface non-linearities such as those produced by radiation damage, surface relaxation, surface roughness, etc. Typically, the Heat of Sublimation is a good estimate of this energy. For single element targets, TRIM will default to a table of energies for each element. This value can be viewed using the Periodic Table of Elements using the button PT, which will also show the values for nearby elements. During a specialized sputtering calculation, special plots are available on the Menu of Plots to show you what effect small changes of the surface binding energy will have on sputtering yield.

- **Lattice Binding Energy** - This is the energy that every recoiling target atoms loses when it leaves its lattice site and recoils in the target. Typically it is about 1 - 3 eV, but values are not known for most compounds. This energy is assumed to go into phonons. The lattice binding energy is, unfortunately, also significant in calculating sputtering yield. Changing the binding energy from 1 to 3 eV may lower the sputtering yield by up to 2x (see section on *"The Physics of Sputtering"*).

Calculation Parameters

"Viewing Window" *for Data and Plotting* – Although TRIM uses the entire target depth to generate averages such as projected range, vacancies per ion, etc., it is possible to enlarge one portion of the target for detailed analysis This is TRIM's *Viewing Window*. For thick targets, this is an important consideration. The depth window allows TRIM to expand a small depth region in the target for fine detail. For example, in the TRIM Demo called "*He (5 MeV) in a Gas Ionization Detector*" the target is 50mm deep. However, the *Viewing Window* is set at 40mm-50mm, allowing more detailed analysis of the end-of-range of the He ions for both the plots and the datafiles. TRIM divides this window into 100 equal-depth bins and stores in them the averaged data for the calculation, for example the energy loss to ionization and the final ion ranges. As another example, in the DEMO section of the TRIM Setup Window, one selection is for 10 MeV H into Be, which has a range of almost 8 mm. For this DEMO, the depth window is set at 7.99 - 8.00 mm. This allows you to see on the plot the detailed collisions at just the final end of each ion's path, and also to have the final collision details in depth segments of 0.1 μm. The *Viewing Window* is set in the TRIM Setup Window, under "*Plotting Window Depths*". The default is zero, which means TRIM will use the total target depth for its stored data. If you input a Depth Window that results in bins smaller than a single atomic monolayer, you will be given a warning that this was requested (e.g. a depth window of 100Å will make data-bins of 1 Å, less than any target monolayer). Requesting a window depth less than 100 monolayers may result is distortions near the layer edges. TRIM defines a monolayer as the inverse cube root of the atomic density of a layer, $N^{-1/3}$, where the

density, N, has units of atoms/cm^3. Hence silicon, with a density of 5×10^{22} atoms/cm^3, has a layer thickness of $(5\times10^{22})^{-1/3} = 2.7$ Å.

- **Number of Ions** - This allows you to set the number of ions which will be calculated. The number can go up to 9999999 ions (which has been requested by several strange users). Normally, you select the default (99999) and interrupt TRIM when it has adequate statistics. Some users wish to stop after a selected number of ions so that different TRIM calculations may be directly compared. If you repeat a TRIM calculation, every ion will be identical to that of a previous calculation unless you change the random number seed (discussed below). If you complete a calculation (finish all ions requested) you can continue this calculation by using the button *Resume Saved TRIM Calc*. Then increase the total number of ions to be calculated.

- **Automatic Saving of Calculations** - Since some TRIM calculations may take days, this allows TRIM to automatically save itself at intervals. You may change this number during the calculation. It may range from 1 - 32000.

- **Random Number Seed** - TRIM will always produce identical calculations (with the same input setup) unless this number is changed. You may input any integer number from 0 - 999999999. The default is set at **716381** which is an almost mystical number in random number theory, and is better than any other number that you will come up with (see Fishman & Moore, S.I.A.M.- J.S.C., vol. 7, 24 (1986)). However, if you want to have three similar but different calculations, then changing the seed from 1 to 2 to 3 will do nicely. The actual random number generator in TRIM is adapted from: P. L'Ecuyer, C.A.C.M., vol. 31, 742-749, 774-776 (1988), "An Efficient and Portable Combined Random Number Generator". At the bottom-right of the TRIM calculation window is a counter of the number of random-numbers used. For calculations with large recoils, this number grows rapidly and may exceed 2^{31} for less than 1000 ions.

Output Disk Files

All of TRIM output files may be declared either from the TRIM Setup window, or requested during the calculation. The advantage of declaring these files in the Setup window is that they start recording from the first ion. These files are explained in much more detail in Chapter 9, TRIM Output Files, and they will be briefly noted here.

- **Backscattered / Transmitted / Sputtered Atoms** - This activates the datafiles for individual ion statistics so that the information about the kinetics of every ion Backscattered or Transmitted, or every target atom Transmitted or Sputtered, is recorded. These files may also be toggled on or off during the calculation by clearing the check-marks beside these requests in the TRIM Calculation window. See the section *"Files of Individual Ion or Recoil Atom Kinetics"* and Chapter 9.

- **Recoil Collision File** - This activates the datafiles for every ion / atom collision which leads to a displaced atom. This file can get big quite fast and should be used carefully (1000 collisions will take up about 64 kB of disk space). In some cases with large cascades, a single ion will generate >1 MB of data). See section *Files of Individual Ion or Recoil Atom Kinetics*, and the extensive notes in Chapter 9.

Scientific Terms used in TRIM

Physics of Recoil Cascades

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:

Displacements = Vacancies + 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:

Vacancies = Interstitials + (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).

Physics of Sputtering

Sputtering is the removal of near-surface atoms from the target. When a cascade gives a target atom an energy greater than the "surface binding energy" of that target, the atom may be sputtered. To actually be sputtered, the atom's energy normal to the surface must still be above the surface binding energy when it crosses the plane of the surface. The sputtering of a surface is described by a "Sputtering Yield", which is defined as the mean number of sputtered target atoms per incident ion. If the target is made of several elements, there is a separate sputtering yield for each element.

The surface binding energy (SBE) of an atom to a surface is known only for a few materials, but it is common to use the heat of sublimation as an estimate. Typical values are: Ni (4.46 eV), Cu (3.52 eV), Pd (3.91 eV), Ag (2.97 eV), Pt (5.86 eV) and Au (3.80 eV). Values will be suggested when you set up the TRIM calculation.

One may calculate sputtering by setting up a normal TRIM calculation with *Full Damage Cascades*. By asking for the data file SPUTTER.txt, a description will be made of each sputtered atom. This request can be made either in the TRIM setup program or during the TRIM Calculation.

Only the cascades which reach back to the target surface are important to sputtering, so it is usually adequate to use only a thin target to simulate sputtering. For heavy ions, e.g. heavier than 20 amu, a target thickness of 40 Å to 50 Å is usually adequate. Using a very thin target reduces the time spent calculating cascades which will not contribute to sputtering. For light ions, e.g. He, it will be necessary to use thicker targets, as much as 300 - 500 Å, since these ions may backscatter from deeper in the target and cause sputtering as they exit from the target surface. The target depth needed for a calculation may be estimated by running several quick cases and seeing for which target depth the sputtering yield remains constant.

For cascades within the target at very low energy (which is a major contributor to sputtering) we use the hard-sphere model for scattering as described in J. P. Biersack and W. Eckstein, Appl. Phys., A34, 73-94 (1984). See figure 3 of this paper, for example.

A final word of caution about Sputtering Yields. The sputtering yield is very sensitive to the surface binding energy (SBE) which you input to the calculation. Be aware that for real surfaces, this changes under bombardment due to surface roughness, and also changes due to surface stoichiometry for compounds. Further, sputtering involves mostly the upper monolayer of the target. For targets such as Ni, or heavier, the electronic energy loss of a target atom moving through the last monolayer is of the order of the surface binding energy, so even monolayer roughness will change the sputtering yield.

The sensitivity of sputtering yield to surface binding energy may be displayed during the calculation by using the plotting menu of *Integral Sputtering* and *Differential Sputtering*.

The Stopping of Ions in Compounds

(See Chapter 5 for an extended discussion of this subject)

A large dictionary of COMPOUNDS has been integrated into the SRIM setup programs. The stopping of ions in compounds is executed using the formalism described in "*The Stopping of Ions in Compounds*", by J. F. Ziegler and J. M. Manoyan, published in Nuclear Instruments and Methods, Vol. B35, 215-228 (1989). The dictionary of compounds can be accessed from the programs by pressing "*Compound Dictionary*".

About 300+ compounds are described in the SRIM Compound Dictionary. You may add other compounds by editing the file *../Data/COMPOUND.DAT*. At the top of this file are instructions about how the dictionary is constructed, and then the dictionary shows its 300+ examples. You will need to know not only the composition of the compound, but also the chemical bonding state of the light elements such as H, C, N, and O. It is easiest to find a compound in the dictionary which closely resembles your new compound, and just alter the parts of this definition.

For a review of the stopping of H and He in compounds, see the review in the report: ICRU Report #49 (ISBN 0-913394-47-5), International Commission on Radiation Units and Measurements, 7910 Woodmont Ave., Bethesda, MD, 20814, USA. Note that the values quoted in this reference as being from *TRIM* or *Ziegler* are from 1977, and are not representative of current SRIM values.

Stopping Powers for Ions in Gases

(See Chapter 5 for an extended discussion of this subject)

TRIM calculates special stopping powers for ions in gas targets of H, He, N, O, Ne, Ar, Kr and Xe. Any gas targets of elements other than those in the above list are treated as solids. This does not mean that the target phase-state is not important. For example, measurements of the stopping of H in Zn, comparing stopping in gas and solid phases, shows 50% stopping differences for ion energies below 100 keV (see references below).

The difference in the ion stopping of gases vs. solids is primarily due to three effects. In a solid, especially a metal, the electrons may form a continuous cloud of mobile conduction electrons which can interact with the ion collectively. Also, the ion will interact with successive atoms very quickly, and excitations of its own electrons may not relax before a subsequent collision. Finally, the ion's polarization of the target electrons will shield the ion from having distant collisions (the polarization effectively decreases the ion's charge state for distant collisions).. In general, the stopping of ions in a solid is lower than for the equivalent gas target (measured by transiting the same number of atoms/cm^2) because of the shielding of the ion by the polarized electrons in the solid. Experiments have shown that both the stopping of ions, and the ion charge state, will vary with gas pressure

The difference between the stopping of ions in gas versus solid targets of H, He, N, O, Ne, Ar, Kr and Xe is only important at low ion velocities. For ions above 200 keV/amu, their stopping powers in solid and gas targets of the same element differ by less than 10%. Below this energy, the difference may reach almost a factor of two. See reference below (Z & M) as to how TRIM treats the differences.

If you ask TRIM for the stopping of ions in gases of compounds, e. g. CO_2, it will use gaseous stopping powers for O (which is in the above gas list) and stopping powers for gaseous C. If you ask for stopping in solid targets of CO_2, you will get stopping for solid C and for solid O added together. If you use the *Table of Compounds*, you can select CO_2 from the table and obtain chemical binding corrections to the stopping of both C and O (see section "*The Stopping of Ions in Compounds*").

For heavy ions, Li - U, there is little data about stopping differences between solids and gases. For these ions, TRIM assumes similar phase differences as for H and He ions in the same targets.

The stopping of ions in gases is very dependent on the gas pressure. One may find stopping differences of more than a factor of two for pressures other than STP (0° C, 760 mm). This difference is especially true for gas densities greater than STP, i.e. several atmospheres. TRIM always assumes a gas target is at STP.

- The phase effect (gas vs. solid target) on stopping powers is of long interest, and one might begin a study of this subject with the excellent ancient paper: W. Mechbach and S. K. Allison, Phys. Rev. *132*, 294 (1963).
- There is no recent review paper which covers all of the above physics. For a discussion of current insights into the phase-effect on stopping powers of ions in materials, see P. Bauer, F. Kastner, A Arnau, A. Salin, P. D. Fainstein, V. H. Ponce and P. M. Echenique, Phys. Rev Lett, *69*, 1137 (1992), or G. Schiwietz, Phys. Rev. *42A*, 296, (1990).
- For details of solid/gas calculations in TRIM, see J. F. Ziegler and J. M. Manoyan, Nuclear Inst. and Meth., *B35*, 215-228 (1989).
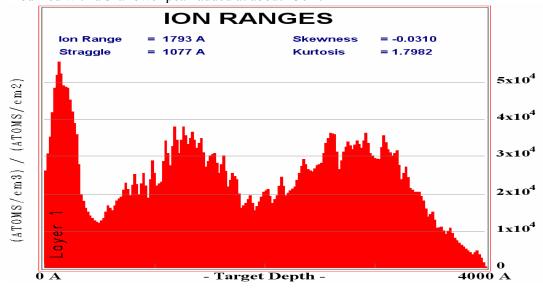
Special Applications of TRIM

Adding Multiple Ions/ Energies/Angles to Same Calculation

During the TRIM calculation, it is possible to merge multiple calculations into one set of datafiles. For example, in the semiconductor industry one might want to make a "triple well" structure, which is very common in CMOS integrated circuit processing. This might require two implants of boron at different energies and doses and one implant of indium into the silicon substrate. It may be that one of these implants is at an angle, 45°, to prevent a phenomenon called "side-wall shadowing". This kind of implant can be easily simulated using TRIM.

Assume that three implants are required at 80 keV, 30 keV and 5 keV, with the 5 keV Indium ion implant being at 45°. For convenience, assume that all three implants will have the same dose.

- Start the first calculation for Boron ions (80 keV) into a silicon (4000A) target.
- When there are adequate statistics for the ion distribution, say at 1000 ions, press the button at the top of the TRIM Calculation window Pause TRIM.
- You can now look at the Ion Distribution plot to see if it is adequate. You will see a broad peak with a range of about 2600Å.
- Press the button Change TRIM .The Ion data window will turn yellow. Change the Ion Energy to 30 keV. Then Press End Edit.
- A window will pop up indicating that the Ion Data has changed. It will ask if you want to add to the existing calculation (YES) or restart the TRIM calculation (NO). Press the YES key.
- Press the Continue button to resume the TRIM calculation, with the boron ions now at 30 keV.
- After another set of ions, press Pause TRIM. You will see that the original deep peak has been modified with a shallower peak added at about 1700Å.
- Press the button Change TRIM .The Ion data window will turn yellow. Change the Ion to Indium (pressing the Ion button brings up the Periodic Table). Change the Ion Energy to 5 keV. Change the Ion Angle to 45. Then Press End Edit.
- A window will pop up indicating that the Ion Data has changed. It will ask if you want to add to the existing calculation (YES) or restart the TRIM calculation (NO). Press the YES key.
- Press the Continue button to resume the TRIM calculation, but with the Indium ions at 5 keV.
- After another group of ions, press Pause TRIM. You will see that the original two peaks have been modified with a shallower peak added at about 130Å.

Using file TRIM.DAT to make Complex TRIM Calculations

Calculating Plasma Ions Hitting a Solid (TRIM.DAT)
Simulating a Receding Surface from Sputtering (TRIM.DAT)
Simulating Reactor Radiation Damage in Metals (TRIM.DAT)

Sometimes users wish to consider incident ions with various energies, with various angles of incidence and possibly starting at various depths. For this application the data file, ***TRIM.DAT,*** is used, see Table 8-1 below. It can be used to simulate the ions from a plasma hitting a surface (various angles and energies), e.g. solar wind effects on planetary materials. It can be used to simulate a receding surface with subsequent ions starting at increasing depths, e.g. from ion sputtering effects. Or it can be used to simulate nuclear reaction processes, e.g. neutron induced alpha-particles created throughout reactor materials. Examples of the control file, TRIM.DAT, can be found in the SRIM directory: ***../SRIM Tools***.

Note: See also the application (later in this chapter):
      Radiation Damage from Neutrons/ Electrons/ Photons (TRIM.DAT)

The top of file ***TRIM.DAT*** contains 10 lines of comments, which are not used in the TRIM calculation. (Ignore the special fonts used in the Table for emphasis; the data file on the disk will be in simple ASCII format.) One of the data lines, as noted in the sample file, will be included as an identifying comment in all output files (named *.txt) which tabulates the statistics of each collision. This is the line: ***Ar Plasma Ions into Si (1000A thick) (Energies 20-80 keV, Various Angles).***

Table 8-1- TRIM.DAT - Sample File for Varying Energy/ Angle/ Depth

TRIM.DAT: TRIM - various Incident Ion Energies/Angles and Depths

Comment: ***Top 10 lines*** are user comments, with line #8 describing experiment.
Comment: ***Line #8*** will be written into all TRIM output files (various files: *.txt).
Comment: ***Data Table*** line consist of: EventName(5 char.) + 8 numbers separated by spaces.
Comment: The Event Name consists of any 5 characters to identify that line.
Comment: Typical Data File is shown below, with a variety of numerical formats, all acceptable.
Comment: Note: $\cos(X) = 1$ for normal incidence; $\cos(X) = -1$ for back towards the target surface.

Ar Plasma Ions into Si (1000A thick) (Energies 20-80 keV, Various Angles)

Event Name	Atom Numb	Energy (eV)	Depth X (Å)	-Lateral-Position- Y (Å)	Z (Å)	------- Atom Direction ------- Cos(X)	Cos(Y)	Cos(Z)
A-1	18	12345	0	0	0	1.00000	.000000	-.000000
abcde	18	54321	0	0	0	0.62344	-.295513	.003415
AA#1	18	1.31E4	123	0	-154	0.34234	-.336437	-.017437
C-3	18	123.55	1230	432	12.3E2	-0.23258	-.543453	.443483
AA-1	18	0.123E2	0	-10	-12	0.99998	.000012	-.000017

Table 8-1 shows the data format for several ions using various numerical styles to show how to specify numbers (all are acceptable). The numbers must be separated by spaces or commas. The first column, called *Event Name*, is a five character ID which will be displayed on the screen while that ion is active. Columns 2-3 show the ion atomic number and energy (eV). Column 4 indicates the depth (Å) in the target where the ion begins: (its x-axis coordinate). The depth must be a positive number. Columns 5-6 are the initial lateral position (Y and Z axis coordinate) of the ion

(Å). TRIM normally uses (0,0,0) as the starting coordinates of the ion. The ion's starting position is always randomly modified within an atomic diameter so that successive ions starting, for example, at (0,0,0) will not have the same impact parameter with a target surface atom. The incident angle of the ion is specified by its directional cosines, columns 7-9, with the x-axis corresponding to depth into the target. For normal incidence, the three directional cosines are: 1,0,0. Note that $\cos(X)$ is positive when the ion is going into the target, and negative when moving towards the target surface. The TRIM.DAT file may be up to 99999 lines long. If any illegal input values are discovered, an error message is displayed on the screen and that input line is skipped.

Important NOTE: TRIM expects that each line of TRIM.DAT ends with two ASCII symbols #13(CR) + #10 (LF). These symbols date back to the teletype era, and mean: CR = Carriage Return, LF = Line Feed. All simple computer editors use this convention, but advanced programs like MS-Word do not. So if you get an error, especially "Illegal Data Line" then you probably need to try another editor to format the file TRIM.DAT.
A second requirement is that at the *TRIM.DAT* data, there must be an **EOF** character (**EOF** = End Of File). Most editors do this automatically and these characters are essential. ***If you finish your calculation and suddenly get* Error #62*, then your data file is missing the EOF character.***

As an example, a file TRIM1.DAT is included in the SRIM directory: ***../SRIM Tools***. This file contains data similar to that shown in the box above for Ar ions (20-80 keV) incident on a Si target (1000 Å thick) To illustrate various modes, this file starts the ions at different angles and at different depths in the target. To use this file to make a TRIM calculation, do the following:

1) Using Windows Explorer, copy *TRIM1.DAT* and paste it into a new file, *TRIM.DAT*. This will create the control file TRIM.DAT out of the above TRIM1.DAT demo file. Put this file into the root SRIM directory (which holds the program TRIM.exe).

2) Start SRIM normally. Select *TRIM Calculation*, which opens the *TRIM Setup* window.

3) In the DAMAGE menu window (upper right) you may specify either the 4th item (quick damage) or the 5th item (full cascade) in the list, "*Varying Ion Energy/Angle/Position using TRIM.DAT*". For this example use the 5th item, *Full Cascades*.

4) Enter the ion type, mass and energy for **Ar** ions at **80 keV**. Note that you must use, for the ion energy, the maximum energy of ions which occurs in the TRIM.DAT file, column 3.

5) Specify for the first Target Atom the element **Si** .

6) Specify **1000** Angstroms for the depth of Layer #1.

7) Specify the stoichiometry as Si = **1** . (default).

8) Use the defaults to specify target density and description (**2.32** g/cm2 and **Silicon**).

9) Specify no other layers.

10) The rest of the questions of the TRIM setup program are optional.

11) Finally, press *"Save Input & Run TRIM"*.

12) During the running of TRIM you will see in the top left of the plots the current ion Event Name from the table in TRIM.DAT. On the left side of the screen you will see the ion energy and position.

13) Run TRIM to completion, (a few seconds)

14) When TRIM reaches Ion #4, an **Error window** opens since this ion is declared in TRIM.DAT to start at 1130A while the target is only 1000A thick. This Error is included in this example to show how TRIM reacts to error in the input file. This error shows you the error messages associated with using TRIM.DAT.

15) After 5 ions, the calculation ends..

To run your own calculation, make up a new file TRIM.DAT, then follow the instructions above. You will have to specify your own ion and target. When you prepare the TRIM.DAT file be sure that your editor places **CR+LF** characters at the end of each line, and at the end of the file there is an **EOF** character (**EOF** = End Of File). These characters are essential. *If you finish your calculation and suddenly get* **Error #62***, then your data file is missing the EOF character.*

This application of TRIM was suggested by: K. Bodek, PSI, Switzerland, F. Calvino, Barcelona, Spain and many others.

Radiation Damage from Neutrons/Electrons/Photons (TRIM.DAT)

TRIM can be used to calculate the recoil cascades in solids caused by neutrons, electrons or photons (which we will call NEP particles). These cases are treated identically, with TRIM evaluating only cascade damage without any incident particle damage.

One must first obtain another computer program for the transport of NEP particles through matter. Widely used codes are the "Integrated TIGER Series", (ITS code) for electrons and photons, or the "Monte Carlo Neutron Program" (MCNP code) for neutrons in matter. Both are available from the Radiation Shielding Information Center, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN, 37831-6362, USA, telephone: (01)-615-5746176, Fax: (01)-615-574-6182, Internet: http://rsicc.ornl.gov. The separate NEP transport programs are used to calculate where collisions are made in the target, and give the position, and recoil statistics for each collision atom. Then TRIM can be used to calculate the full target recoil cascade which occurs from each NEP collision atom.

A file called **TRIM.DAT** must be prepared by the user which specifies the parameters of each cascade. An example of **TRIM.DAT** is shown in Table 8-2 and included in SRIM as *../SRIM Tools/TRIM2.DAT.* TRIM calculates the cascades with an "invisible" incident particle. TRIM.DAT specifies each recoil atom and TRIM calculates its cascade.

Table 8-2 - *TRIM.DAT* - Sample File for Collision Cascades

TRIM.DAT : TRIM recoil cascade data file								
Comment: **Top 10 lines** are user comments, with line #8 describing experiment.								
Comment: **Line #8** will be written into all TRIM output files (various files: *.txt).								
Comment: **Data Table** consists of: EventName(5 char.) + 9 numbers separated by spaces.								
Comment: The Event Name consists of any 5 characters to identify that line.								
Comment: Typical Data File is shown below, with a variety of numerical formats, all acceptable.								
Comment: Note: cos(X) = 1 for normal incidence; cos(X) = -1 for back towards the target surface.								
Recoils from 1670000 eV electrons in SiO2(1200A)+GaAs(10000A)								
Event Name	**Atom Numb**	**Energy (eV)**	**Depth X (Å)**	-Lateral-Position- Y (Å)	Z (Å)	------- Atom Direction ------- Cos(X)	Cos(Y)	Cos(Z)
A-1	8	59.2	322	24	12.34	0.99998	.000012	-.000017
C-3	33	1259.	10.02E3	432	12.3E2	-0.23258	-.543453	.443483
AA-1	8	98764	522	-24.3	-12	0.99998	.000012	-.000017
123C	14	1.56E4	2222	-33	-69	0.62344	-.295513	.003415
9875	33	7.31E4	3322	-82.9	154	0.34234	-.336437	-.017437
asd	6	0.98E5	0.882E2	-206	588	0.03754	.032936	-.334616

The top of file **TRIM.DAT** contains 10 lines of comments, which are not used in the TRIM calculation. (Ignore the special fonts used in the Table for emphasis; the data file on the disk is in simple ASCII format.) One of the data lines, as noted in the sample file, will be included as an identifying comment in the file **COLLISON.txt** which tabulates the statistics of each collision (This is the line: "*Recoils from 1670000 eV electrons in SiO2(1200* Å)+ *GaAs(10000* Å)"). The important numerical data at the bottom of the file may be written in several different formats, such as 12345, 12.345E3, 0.12345E5, etc.

Table 8-2 shows the data for several recoils using various formats to show how to specify numbers. The numbers must be separated by spaces or commas. The first data column, *Event Name*, is a five character ID which will be displayed on the screen while that recoil is active. Columns 2-3 show the recoiling atom atomic number and energy (eV). Column 4 indicates the depth (Å) in the target where the recoil atom starts- this is the x-axis coordinate. The depth must be a positive number. Columns 5-6 are the initial lateral position of the atom (Å). The initial trajectory of the recoiling atom is specified by its directional cosines, columns 7-9, with the x-axis corresponding to depth into the target. For a recoil trajectory normal to the target surface, the three directional cosines would be: $\cos(X)=1$, $\cos(Y)=0$, $\cos(Z)=0$. Note that $\cos(X)$ is positive when the ion is going into the target, and negative when moving towards the target surface. The TRIM.DAT file may be up to 99999 lines long. If any illegal input values are discovered, an error message is displayed on the screen and that input line is skipped.

The sample input data file shown in Table 8-2 is for 1.67 MeV electrons into a target of SiO_2 (1200 Å) on GaAs (10000 Å). If you wish to try TRIM using the sample data file **,** follow these steps:

- Using Windows Explorer, copy *TRIM2.DAT* and paste it into a new file, *TRIM.DAT* in the root SRIM directory. This will create the control file TRIM.DAT out of the above TRIM2.DAT demo file. The file must be in the same directory as **TRIM.exe**.
- Start TRIM normally and select *TRIM Calculation* to go to the TRIM Setup window.
- In the DAMAGE menu (upper right) specify either the 6^h item (quick damage) or the 7^h item (full cascade) in the list, "*Damage cascades from neutrons, using TRIM.DAT*". For this example, choose the 7^h item: "*Damage Cascades from Neutrons, etc. (Full Cascades) using TRIM.DAT*"
- For the ion Type and Mass use any values since **this data is not used**. For this calculation, there is no ion, only recoils. So in this example, for electron irradiation, you can still get the full target damage even though SRIM can not normally be used for beams of electrons.
- For the *Ion Energy*, specify the maximum energy which occurs in column 3 in *TRIM.DAT*. For the data shown in Table 8-2, you use 100 keV. This will assure that stopping powers are calculated for all recoils up to this energy.
- You will make a target with atoms of **Si**, **O**, **Ga** and **As** (You must specify every atom noted in column 2 of the TRIM.DAT file, and this atom must exist at the depth noted in column 4. Otherwise, you will get an error message on the screen, and this event will be omitted.)
- Specify that the target first layer with a depth of **1200** Å and containing **Si(1)+O(2).** TRIM normalizes the stoichiometry so you may use any equivalent units such as **Si(33)+O(66).** The second target layer has a layer depth of **10000** Å and is composed of **Ga(1)+ As(1).** There is no third target layer.
- Finally, press "**Save Input & Run TRIM**".
- You may get a window asking if you want to generate the file *COLLISON.txt*. Answer "**No**"
- During the cascade calculation, on the screen you will see small isolated pockets of damage, with no intermediate ion tracks. The TRIM damage plots may be accessed normally at any

time. The cascade results will be stored in **COLLISON.txt** if you answered "Yes" in the above step. You may interrupt the calculation at any time, and continue it later (TRIM will start where it left off).

When you prepare the ***TRIM.DAT*** file be sure that your editor places **CR+LF** characters at the end of each line, and at the end of the file there is an **EOF** character (**EOF** = End Of File). Most editors do this automatically and these characters are essential. If you finish your calculation and suddenly get Error #62, then your data file is missing the EOF character.

NOTE: TRIM will assume that each *Event Name* data row in TRIM.DAT comes from a different incident particle, and hence its statistical averages will be in error for cases where a single particle may cause several recoils, e.g. for a high energy neutron may cause several *Event* data lines in TRIM.DAT. To correct for this counting error, take the calculated TRIM statistical averages and multiply by ($N_{Events}/N_{Particles}$). For example, if the TRIM.DAT file contains 100 events caused by 20 incident particles, then every average needs to be corrected by multiplying by (100/20) = 5. So if the TRIM output shows "*Vacancies/Ion = 10*" the corrected average value would be 50 Vacancies/Particle.

As with normal runs of TRIM, the calculation may be interrupted and saved at any time. When TRIM resumes, it will automatically skip cascades which have been previously calculated.

COLLISON.txt contains the data on every ion/target collision which exchanges enough energy to produce a vacancy (energy above the Displacement Energy). This file can get quite large. If the data file is turned off, then on again, further data may be appended to the old data. (See section on TRIM Execution and Commands in Chapter 9 on ***TRIM Outputs***.)

The above instructions were suggested by R. Macaulay-Newcombe of McMaster Univ.; Canada; and M. Robbins, Univ. of West London, UK; and F. Calvino, Barcelona, Spain).

Special Setup for Multi-Layered Biological Targets

Use the *Compound Dictionary* in the TRIM setup window to use any of the standard ICRU or ICRP biological target specifications. See the following citations for "standard" compounds:

- International Commission on Radiation Units - Report ICRU- 33, "Radiation Quantities and Units", 1980, ICRU, Bethesda, MD, USA.
- International Commission on Radiation Units - Report ICRU- 37, "Stopping Powers for Electrons and Positrons", 1984, ICRU, Bethesda, MD, USA.
- International Commission on Radiation Units - Report ICRU- 49, "Stopping Powers and Ranges for Protons and Alpha Particles", 1993, ICRU, Bethesda, MD, USA.
- H.Q. Woodward and D. R. White, British J. of Radiology, vol. 59, 1209-1219 (1986).

An example of this type of calculation is included in the *Demo* examples available in the TRIM Setup window. If you wish to enlarge or change the *Table of Biological Targets*, you need to edit the file ***../Data/COMPOUND.DAT*** in the SRIM directory. This contains all the data of the biological targets. There are instructions at the top of the file which indicate the data format. In general, each target is described by a line of text, which is displayed in the table-of-contents during layer selection, and a line of data which describes the layer to the TRIM calculation. The table also contains the data for corrections to the ion stopping powers based on chemical binding information,

but this correction is beyond the scope of this manual. Please note that TRIM will accept targets made of up to 12 elements.

This application was suggested by Tammy Utteridge, Royal Adelaide Hospital, Australia, and Wayne Newhauser, PTB, Braunschweig, Germany.

How to Obtain 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 light 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. Below are the steps required to generate the required data. (Note that this procedure may be inaccurate for heavy ions which create significant recoil cascades, whose electron excitation is not included in the ion's electronic energy loss.)

- 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 datafile *../SRIM Outputs/COLLISON.txt*. A sample of this file is described in detail in the Chapter on **TRIM Outputs**. You will see a file like the one shown below:

Table 8-3 - 3-D plots of 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 stopping (rate of energy loss) of the ion to the target, Se, 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 change

smoothly due to Monte Carlo straggling variations. The values of Se oscillate about a mean value because TRIM is applying straggling statistics to this parameter (see Chapter 7 on TRIM Theory). This application was suggested by Lidia Didenko, Univ. of Maryland.

How to use TRIM for Isotopically Enriched Targets

TRIM assumes that a target has the natural abundance of isotopes, e.g. that lithium is made up of 7.5% of Li^6 and 92.5% of Li^7 . To use TRIM with isotopically enriched targets, it is necessary to follow the steps below (using the example of an enriched target with 90% Li^6 and 10% Li^7) :

During the TRIM setup program, for the target atoms declare ***Li*** twice. Then declare the mass of one to be 6 with a stoich of 90, and the other with a mass of 7 and a stoich of 10. (For elements with more isotopes, you may specify the element up to twelve times, for up to twelve isotopes.)

Straggling in Ion Energy Reducers (Energy Degraders)

TRIM may be used to calculate the energy loss through foils or thick blocks of materials used to lower the energy of a beam of particles. This is often done for light ions, such as protons, to obtain lower energies quickly. For example, if one starts with a beam of monoenergetic protons at 158.6 MeV and introduces a block of plexiglas (called *perspex* in Europe, and Japan) 14.1 cm thick, the exiting beam of particles will be at 30 MeV. Degrader blocks made with light atoms can reduce particle energy with a minimum of straggle and little long term radioactivity (plexiglas is $C_6H_4O_2$).

Two problems occur in planning "energy degraders". First is the calculation of the proper block thickness, and second is the calculation of the final beam energy spread. Below we illustrate both calculations.

The calculation of the required degrader thickness consists of four basic steps. We illustrate these steps below using the example of protons being slowed by a block of plexiglas from an initial energy of 158.6 MeV to a final energy of 30 MeV.

1   Make a table of proton stopping in plexiglas by executing the program Table of Stopping and Range of Ions using the SRIM Title Menu. In the program, select a target of plexiglas in the Table of Compounds and then generate a stopping/range table for protons up to 160 MeV in plexiglas, with the stopping powers specified in units of MeV/mm.

2   Using the table generated in (1), find the range of protons for the initial beam energy and estimate the depth at which the protons will be at 30 MeV by looking at the ranges and working backwards. For example, the table will show that 160 MeV protons have a range of 154.54mm in plexiglas, and 30 MeV protons will go 7.63mm. Hence your first guess for the thickness of plexiglas to reduce 160 MeV protons to 30 MeV will be 154.54 - 7.63 = 146.9 mm thick. Further, since the initial proton beam is not 160 MeV but 158.6 MeV, one interpolates the distance protons travel between 160 MeV to 158.6 MeV as 2.30 mm, so the initial block size for an incident 158.6 MeV beam will be 146.9 - 2.30 = 144.6 mm. Setup TRIM for protons in plexiglas at this thickness. Be sure to set the flag to store the energy spectrum of the *Transmitted Ions*, which will create the file TRANSMIT.txt that contains all the kinetic details about the transmitted ions.

3   Execute TRIM to get a file of transmitted ions. You now need to execute a program to analyze these results. SRIM includes a BASIC program, *../SRIM Tools/TRANSMIT.BAS*, which will analyze the transmitted particles which TRIM stores in the file TRANSMIT.txt. This program will give you both the mean final energy and the energy straggling of the transmitted protons.

This program is written in BASIC so that you can look at the source code and modify it for your needs. (You can easily generate your own code, since the datafile is simple to read.)

4 Use the difference between your desired final energy (30 MeV) and mean final energy found in step 3 above, along with the stopping power tables, made in step 1 above, to estimate a new target thickness. For example, if the protons exit at 32 MeV and the stopping power for protons at 30 MeV is 2.16 MeV/mm, then you need (2 MeV)/(2.16 MeV/mm) = 0.92 mm more plexiglas in the block to bring the beam down to 30 MeV. Use the TRIM setup program with "*Restore Last TRIM Data*" to make up a new plexiglas target with a width of 144.6 mm (initial estimate) + 0.92 mm (correction) = 145.52 mm. Loop through steps 2-4 until you come get as close as you want to the desired thickness.

The final energy straggle of the beam after it has passed through the energy reducing block is a mixture of two components: (1) the straggle introduced by random collisions in the degrader block and (2) the broadening of any incident beam energy straggle by the block (straggle is the spread of the ion beam energy spectrum). We calculate the straggle of the incident monoenergetic beam with the TRIM calculations above, steps 1-4, and we find, for example, a straggle of about 2.0 MeV when we degrade protons from 160 MeV to 30 MeV using plexiglas (this comes out of the analysis program TRANSMIT.BAS). To this broadening, we have to add the straggle due to expansion of the initial beam energy spread, which may be the dominant factor in the final energy width. Assuming that the incident beam is not monoenergetic, but has a spread of 1 MeV at 160 MeV, we will find that this spread expands to 3.6 MeV by the time the beam degrades to 30 MeV. This expansion occurs because of the non-linearity of stopping powers with particle energy as explained below.

Assume that the energy straggle of the incident beam is σ. We show below that the final energy straggle of the exiting beam, σ', can be estimated as :

$$\sigma' = (S'/S) \, \sigma ,$$

where S and S' are the stopping powers, dE/dx, in the degrader material at the initial and final beam energy.

Consider two particles of the incident beam with energies E_1 and E_2, separated by the incident beam energy straggle, σ. The final energy straggle of these two particles, after transiting the energy-lowering block of material, is defined as $\sigma' = E_1' - E_2'$. where E_1' and E_2' are the final energies of particles 1 and 2.

Considering the incident particles, assuming $E_1 > E_2$, then particle #1 will travel a short distance into the degrader block before its energy will be reduced to that of particle #2. This distance, x, is about $x = \sigma / S$, where S is the particle stopping power (dE/dx) at energy E. After particle #1 reaches depth x, then both particles #1 and #2 will transit through the block similarly until particle #1 reaches the end of the block. Particle #2 will still have more of the block to traverse, an amount $x' = \sigma' / S'$, where $\sigma' = E_1' - E_2'$, the final energy difference between the two particles, and S' is the stopping power at the final beam energy, E'. But the block length is the same for both particles, so $x = x'$, and therefore $\sigma / S = \sigma' / S'$. This can be solved for the energy straggle, $\sigma' = (S'/S) \, \sigma$ **.**

Note that several approximations are made in this argument, especially that $S(E_1) = S(E_2)$ and $S(E_1') = S(E_2')$, and that the total energy loss is much larger than the straggling, $(E - E') \gg \sigma$.

For an example, protons at 160 MeV in plexiglas have a stopping power of 0.593 MeV/mm and at 30 MeV have a stopping power of 2.157 MeV/mm. Assuming the initial beam straggle, σ, is 1

MeV, then the final beam energy straggle, σ' = (1 MeV) (2.157 MeV/mm) / (.593 MeV/mm) = 3.6 MeV.

The total beam spread through the energy-degrader block is the rms total value of two separate quantities : (1) the beam straggle through the block, 2.0 MeV, and (2) the beam energy broadening due to non-linear stopping powers, 3.6 MeV, which, when added in quadrature, gives a total straggle of 4.1 MeV .when protons at 160 MeV are degraded to 30 MeV.

The above comments come from Dr. Bernard Gottschalk, Harvard Cyclotron Laboratory, Harvard University, USA.

Getting High-Resolution Collision Data from TRIM

TRIM breaks the target into 100 equal-depth layers, each parallel to the surface. These layers are defined by the **V***iewing Window*, i.e. the depths that you see on your screen during the calculation. For example, if you try the DEMO (from the TRIM Setup window) of 10 MeV protons into Be, you will find that the target is defined down to 1000 μm, but the viewing screen is defined as the 800-900 μm depth in the target. The collision data (vacancies, displacements, ion ranges, etc.) are stored in 1 μm bins from 800 to 900 μm. You can get data in 1μm bins for the whole 1000 μm target depth by repeating the calculation with different viewing windows, and saving each set of data files separately. That is, repeat the same calculation for viewing depths of 0-100 μm, 100-200 μm, etc., each time storing the data separately. When TRIM repeats a calculation, it calculates exactly the same ions which follow the same trajectories and which have the same collisions (unless you explicitly change the random-number seed in the TRIM setup program). So the data you collect in the ten calculations necessary to cover the 0-1000 μm total target thickness will smoothly go together, and you can get 1000 bins, with 1 μm resolution, after ten TRIM runs with the above example.

This suggestion was made by Sarah Clark, Princeton University, USA.

Evaluating the Details of "Ion Mixing" Experiments

TRIM is often used for studying the mixing of similar layers such as NiSi/SiO$_2$/Si. It is sometimes useful to try to identify which layer recoil atoms come from. You can specify different identical atoms for each layer, and TRIM will treat them separately. For the example, you can specify target atoms of **Ni**, **Si**, **Si**, **O** and **Si**. TRIM will treat these as separate atom types, and in plots or in text files they will be separately indexed.

If you wish to examine an interface closely, remember that you can isolate the interface using the *Viewing Window* option in TRIM, and blow up the interface region with monolayer resolution. As an example, assume your target is: NiSi (3000 Å) / SiO$_2$ (2000 Å) / Si (5000 Å). The total target is 10,000 Å thick. But you may specify the *Viewing Window* as 2800 Å to 5200 Å and thereby see the interface with twice the resolution. If you save data in the *.txt files (previously discussed) the data will now be grouped in 24 Å segments instead of 100 Å segments. Note that the TRIM averages (e.g. the range or straggling) are calculated precisely and are not limited by the data segments.

Using TRIM for Mixed Gas/Solid Targets

If you wish to calculate ion stopping in a mixed solid/gas target, for example alpha-particles transmitted through an ionization chamber, you must consider how TRIM stores collision data. TRIM is set up to store the averaged collision results in 100 bins. The bins are equally spaced in

depth, so if you have a thin window, say 10 μm of Al, then 100 mm of gas, then a final layer of 10μm of Al, the TRIM output will be stored in about 1 mm bins. Since these bins are far bigger than the solid 10 μm windows, TRIM stores combined solid and gas collision data in the first and last bins.

There are 3 different ways to get accurate data for all parts of the target:

1. If you care only about the gas-cell part of the target, then set the *viewing window* only for the gas part of the target. TRIM will then set up its 100 bins for this gas layer only (the bins are defined by the viewing window, not by the total target width). In the above example, Al(10μm) + Gas(100 mm) + Al(10μm), your target thickness is 100.02 mm and your viewing window will start at .01 mm and end at 100.01 mm. (Note: TRIM does not use bins in its ion transport calculation, only to store averaged results.) The declaration of the "*Plotting Window Depths*", also called the *Viewing Window*, is part of the TRIM Setup window. See Chapter 12, TRIM Tutorials, #4, for more details.

2. Use the detailed data supplied in the Individual Ion Datafiles. These are described in detail in Chapter 9 , **TRIM Outputs,** which discusses all the possible TRIM datafiles. You can generate a file called COLLISON.txt, which contains all the data of every ion/atom collision, and then extract whatever data that you need. This file can be initiated either in the TRIM setup program by pressing "*Collision Details*" or checking this box during the TRIM calculation

3. Run TRIM for each section separately, e.g. the entrance foil, the gas cell and the exit foil. For each calculation, you will save a file of transmitted ions and use this as input data for the ions into the next layer. This is described in the section on *Ions starting with varying Energies, Angles and Depths.* After each calculation you must rename the collision data files, *.txt, so they are not written over by the next calculation.

Be sure to remember to declare any GAS portions of the target, so that it will be treated correctly as a gas (Chapter 5 discusses the differences in stopping in gases vs. solids).

(Discussion suggested by F. Calvino, Barcelona, Spain)

Datafile of Complete Ion Trajectories through a Target

It is possible to track an ion through the target, storing its position at various points of its path. Doing this for every collision is possible using the special output datafile called ***COLLISON.txt***. . TRIM has various filters for this file to keep it from overwhelming the user with its details. See Chapter 9 for details.

However, it is possible to 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 selection called **"*Special EXYZ* File *Increment (eV)*"** This will generate a datafile of the ion position at specific energies: *../ SRIM Outputs / EXYZ.txt*

There is an example of this command in the **DEMO** menu of this window. The Demo sets up Bi(500 keV) ions into silicon. It is set so that every time the ion loses 25 keV, an entry will be made into the file of the ion's position. That is, the ion's position is stored at energies of about 500 keV, 475 keV, 450 keV, 425 keV.

Table 8-4 shows a typical output of this DEMO calculation. The ion energies are not exactly at the 100 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.

Table 8-4 - Table of 3-D Position of Ion Trajectory in Target

```
========================= SRIM-2006 =================================
 ===================================================================
 =                    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
           Bi     208.98   500 keV    100 keV

 ===================================================================
Ion        Energy      Depth (X)     Y           Z          Energy Lost(eV)
Number     (keV)     (Angstrom)  (Angstrom)  (Angstrom)   Last Collision
-------  ----------   ----------  ----------  ----------   -----------
0000001 5.0000E+05   0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00
0000001 4.9990E+05   4.5634E+03  -7.9972E-01   1.8242E+00   1.8998E+05
0000001 3.9991E+05   4.6482E+04   1.1253E+02   6.4566E+01   1.9992E+05
0000001 2.9992E+05   9.6187E+04   1.1568E+02  -1.2677E+02   9.8713E+04
0000001 2.0000E+05   1.5203E+05  -3.9668E+02  -8.1722E+02   6.6356E+04
0000001 9.9985E+04   2.2324E+05  -7.8673E+02  -1.0863E+03   7.3526E+04
0000002 5.0000E+05   0.0000E+00   0.0000E+00   0.0000E+00   1.2233E+00
0000002 3.9979E+05   4.6043E+04   2.8184E+01   1.0037E+01   2.1920E+05
0000002 2.9992E+05   9.5422E+04   1.6411E+02  -2.3177E+02   1.7898E+05
0000002 1.9995E+05   1.5194E+05  -8.5354E+02  -5.0238E+02   6.6654E+04
0000002 9.9942E+04   2.2295E+05  -1.8743E+03  -2.9341E+02   9.2119E+04
```

TRIM - Common Questions and Solutions

What are "Projected Range" and "Radial Range" Distributions ?

The program assumes that there is cylindrical symmetry in the final ion distributions. The assumed cylindrical axis is perpendicular to the target surface at the point of ion impact. (If the initial ion beam is not normal to the target surface, then none of the following is valid.) The *"radial"* parameters refers to these cylindrical coordinates. The *"projected"* parameters assumes that an X-Y plane has been inserted through the axis, and the final ion distribution is projected onto this plane. This projection is identical to the view on the PC screen and marked as the "XY Plane" (X is the depth axis; the XZ plane is perpendicular to the XY plane).

The mean *"lateral range"* of the ions is zero in both the radial and projected definitions if there is cylindrical symmetry. So the lateral range in TRIM is defined as the mean absolute value of the lateral range. The *"ion straggling"* has its normal definition as the second moment of the distribution. The lateral projected parameters directly describe the final distribution under a mask edge as used in VLSI technology. Remember, the total ion concentration directly at a mask edge is one half of the concentration of a uniform implantation distribution.

What is Straggling, Skewness and Kurtosis ?

These words are names for statistical quantities related to the second, third and forth moments of the ion distribution. They are important because many VLSI modeling programs require these parameters to create analytic functions of ion implantation distributions. The use of these words in the ion implantation field is DIFFERENT from that in some statistics textbooks. In this field, we use mostly the definitions first proposed by B. Winterbon ("Ion Implantation Range and Energy Distributions", vol. 2, Plenum Press, 1975). For convenience, we define each moment below in several different standard notations. It is assumed below that the ion trajectory begins perpendicular to the target surface, co-linear to the x-axis, and the y-axis and z-axis are orthogonal in the target surface plane (during the TRIM calculation, the window "Collision Plots" controls four displays of the ion and recoil trajectories projected on the XY, XZ and the YZ planes).

$$\text{Mean Projected Range} \quad \equiv R_p = \Sigma_i \, x_i / N \quad = <x> .$$

$$\text{Lateral Projected Range} \quad \equiv R_y = \Sigma_i \, |y_i| / N = <|y|> .$$

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

Where x_i is the projected range of ion "i" on the x-axis, i.e. the perpendicular distance from the surface to the end of an ion's track; $\Sigma_i \, x_i$ = sum of the ion projected ranges; $\Sigma_i \, x_i / N$ = the mean projected range of N ions; and $<x>$ = the mean projected range of all ions. The transverse coordinate "y" is treated the same, except the distance is taken in the XY plane. The mean projected lateral range is zero for a perpendicular beam, so the above lateral range definition averages the absolute values to provide other information on the first moment of the radial spread. The mean radial range assumes cylindrical symmetry of the ion distribution.

"Variance" is the second moment of the range distribution, and we show below several identical definitions using various common notations.

$$\text{Variance} \quad = \Sigma_i \, (x_i - R_p)^2 / N \quad = <(x - R_p)^2> ,$$

$$= \Sigma_i \, \Delta x_i^2 / N \quad = <(\Delta x_i)^2> ,$$

$$= <x^2> - <x>^2 \quad = (\Sigma_i \, x_i^2) / N - (R_p)^2 .$$

Where $\Sigma_i \, \Delta x_i^2$ = sum of the square of the deviations of the ion ranges from the mean projected range with $\Delta x_i = (x_i - R_p)$.

"Straggling" is a word which is used in ion implantation in several ways, and care should be taken to determine the author's definition. Sometimes it is a synonym for variance and sometimes it is defined as the square root of the variance. In other cases an author, such as Winterbon, uses normalized definitions such as: Straggling $= <\Delta x_i^2> / <x>^2$. We use the common definition that straggling is the square root of the variance:

$$\text{Straggling} \quad \equiv \sigma \quad = [(\Sigma_i \, x_i^2) / N - R_p^2]^{1/2} \quad = <(\Delta x_i)^2>^{1/2} .$$

$$\text{Radial}$$
$$\text{Straggling} \quad \equiv \sigma_r \quad = [\Sigma_i \, (y_i^2 + z_i^2)/N - R_r^2]^{1/2} = <(\Delta r_i)^2>^{1/2} .$$

We define lateral straggling in the same way as range straggling above. (Lateral coordinates are sometimes called Transverse coordinates.) For a normally incident beam we can assume cylindrical symmetry of the range distribution, so the mean lateral projected range is zero (i.e. $\mathbf{R_y = 0}$) . Further, we average the Y and Z projected ranges to increase statistical accuracy:

Lateral

$$\text{Straggling} \equiv \sigma_y = [\, \Sigma_i \, ((|y_i| + |z_i|)/2)^2 \, / \, N \,]^{1/2} \; .$$

$$\text{Skewness} \; \equiv \gamma \; = \; <\Delta x^3> \, / \, <\Delta x^2>^{3/2} \; ,$$

$$= \; \Sigma_i \, (x_i - R_p)^3 \, / \, (N\sigma^3) \; ,$$

$$= \; \Sigma_i [x_i^3 - 3R_p x_i^2 + 3R_p^2 x_i - R_p^3 \,] \, / \, (N\sigma^3) \; .$$

$$\text{Kurtosis} \equiv \beta \; = \; <\Delta x^4> \, / \, <\Delta x^2>^2 \; ,$$

$$= \; \Sigma_i \, (x_i - R_p)^4 \, / \, (N\sigma^4) \; ,$$

$$= \; \Sigma_i [x_i^4 - 4R_p x_i^3 + 6R_p^2 x_i^2 - 4R_p^3 x_i + R_p^4 \,] \, / \, (N\sigma^4) \; .$$

TRIM uses the last variations shown above for the calculation of skewness and kurtosis.

In the above TRIM definitions, the projected range and the straggling have dimensions of length, while the higher moments, skewness and kurtosis, are dimensionless. Note that we do NOT include backscattered or transmitted ions in our moment calculations, in contrast to some theorists. The skewness tells whether the peak is skewed towards the surface (negative values) or away from the surface (positive values). Another way of stating this is that negative skewness indicates that the most probable depth (the peak position) is greater than the mean depth, and positive values indicate the reverse. Kurtosis indicates the extent of the distribution tails, with a value of 3.0 indicating a Gaussian distribution. Since both the shallow and deep tails contribute, no simple rule indicates what a variation from 3.0 means about the ion distribution. In general, values from 0 to 3 indicate abbreviated tails, and values above 3 indicate broad tails. The papers which most clearly discuss how to regenerate complete distributions from statistical moments are : K. B. Winterbon, A.E.C.L. Reports #4829 (1972) and #4832 (1972), and especially CRNL-1817 (1978), available from the Chalk River Nuclear Laboratory, Chalk River, Ontario, Canada, K0J-1J0.

What Causes Anomalous Peaks and Dips at Layer Edges ?

There are several reasons that small artifacts occur at layer edges, and these are all associated with inconsistencies between two parts of TRIM :

1. The TRIM "*Viewing Window*", which is the portion of the target displayed on the screen, is divided into 100 equal segments or bins. (Your target may be much larger than the data window, but only the collision data within the window is saved. The position of the data window within the target is set in the TRIM input program.)

2. Atoms in a target are not randomly spaced, even in amorphous targets. There is a minimum distance between atoms, and once a collision occurs the ion must travel at least one monolayer to reach the next atom. TRIM defines a monolayer as the inverse cube root of the atomic density of a layer, $N^{-1/3}$, where the density, N, has units of atoms/cm^3. Hence silicon,

with a density of 5×10^{22} atoms/cm^3, has a layer thickness of $(5 \times 10^{22})^{-1/3} = 2.7$ Å. If your layer thickness is not a multiple of this monolayer thickness, there may be a small error at the bottom edge.

An accounting problem occurs when the ion jumps from one layer to another, and TRIM must decide where to place the collision data. Typically, the following conditions cause small problems

- If your target layers do not end exactly at a data bin edge, then that bin consists of two different materials, and TRIM will assume one or the other based on the current ion's trajectory at that bin. When you input a new target, you are warned of this problem if it occurs.
- If a data bin is less than one monolayer wide, then TRIM may not treat it accurately since calculation distances are never smaller than one monolayer. The same occurs to a lesser extent if a thin layer, say 20A wide, is not an integral number of monolayers wide.
- Thin layers at the surface, or at the bottom of a target, may cause problems if ions leave the target. The point where the target ends is not clean if this layer is less than many monolayers thick, since TRIM works in monolayer steps, and the surface appears "smoother" to an ion moving almost parallel to the surface than to one moving perpendicular to the surface. Once the next ion step is found to be outside the target there are no further collisions. So inaccuracies of the order of one monolayer are probable. The special TRIM calculation for sputtering takes special precautions to prevent these errors from occurring at the target surface.

The small dips and peaks may extend more than one data bin at a layer's edge. TRIM runs efficiently because the ion can jump many monolayers between collisions, and the intermediate collisions are approximated. We suggest that you do not worry about small peaks and dips at layer edges, they are not worth the trouble to try to avoid, and just average the final curves.

Running TRIM in Batch mode: TRIM.IN

The input data file which controls the TRIM calculation is called TRIM.IN. It is normally created by the TRIM Setup window. Once you have set up a TRIM calculation, you may wish to only change a few parameters, e.g. the ion's energy and angle for simulation of an ion plasma bombarding a solid surface. You will need to run software which executes a few simple steps as in the following example.

(1) Setup the first TRIM calculation with a fixed "*Number of Total Ions*" = 100 (as an example). This TRIM calculation must specify the highest energy that the ion will have in any subsequent calculation. Run the TRIM calculation until it completes all the ions.

(2) Edit the file TRIM.IN in the SRIM root directory. Change the ion energy and angle. The new energy may not be larger than that of the initial calculation. Increase the total number of ions (line 3) from 100 to 200 to calculate for another 100 ions.

(3) Edit the file *TRIMAUTO* in the SRIM root directory. Replace the "0" in the first line with a "2". This will make TRIM run without any keyboard inputs until it reaches the end of the next calculation (Ions = 100 in this example). It will also add the next calculation results to the previous ones. There is an explanation of this procedure in the file *TRIMAUTO.txt*.

(4) Execute the file TRIM.exe in the SRIM directory. This will run TRIM with the new setup (in this example with a changed ion energy and angle) and add the results to the old calculation results.

(5) Continue with steps 2-4 until you have completed all various of ion energy and angle. TRIM will not require any keyboard inputs during the calculation, so by automating steps 2-4 you will make TRIM sum all the calculations into the standard files, and the plots will show the summed results.

Below are examples of TRIM.IN. Note that the datafile contains lines of comments (which are not

used). The comment lines are show in *Italics*, while the input data are shown in **Bold**. Only the **Bold** items are used by TRIM. The numerical data has free format, with almost all standard formats accepted (e.g. 99 or 99.00 or 99E0 or 0.99E2). This file is also described in detail in Chapter 9.

Table 8-5 - Datafile TRIM.IN for Au(100keV) into Lead(2000Å).

==> SRIM-2006.02 This file controls TRIM Calculations.
Ion: Z1 , M1, Energy (keV), Angle,Number,Bragg Corr,AutoSave Number.
   79   197   100   0   99999   0   100
Cascades(1=No;2=Full;3=Sputt;4-5=Ions;6-7=Neutrons), Random Number Seed, Reminders
          2   **0**   **0**
Diskfiles (0=no,1=yes): Ranges, Backscatt, Transmit, Sputtered, Collisions, Special EXYZ.txt file
                0   **0**   **0**   **0**   **0**   **0**
Target material : Number of Elements & Layers
"Au(100 keV) into Pb (3000 Vacancies/Ion)"   **1**   **1**
PlotType (0-5); Plot Depths: Xmin, Xmax(Ang.) [=0 0 for Viewing Full Target]
   1   **0**   **0**
Target Elements: Z   Mass(amu)
Atom 1 = Pb =   82   208
Layer   Layer Name /   Width Density   Pb(82)
Numb.   Description   (Ang) (g/cm3)   Stoich
 1   **"Lead"**   **2000**   **1.14**   **1**
Target layer phases (0=Solid, 1=Gas)
0
Target Compound Corrections (Bragg)
1
Individual target atom displacement energies (eV)
    21
Individual target atom lattice binding energies (eV)
    2.1
Individual target atom surface binding energies (eV)
    3.1
Stopping Power Version (1=2006, 0=2006)
 0

The above TRIM.IN is obtained by executing the TRIM Setup window, and selecting the DEMO for "*Au (100 keV) in Pb*". In Table 8-5: Note: (This files is explained in much more detail in Ch. 9.)
- Lines 1 and 2 are comments
- Line 3 = the data for the ion, showing atomic number, mass (amu), energy (keV), incident angle to the surface (degrees), Bragg correction to stopping (0=none), and the Autosave number (save calculation after every 100 ions).
- Line 4 is a comment
- Line 5 = Type of calculation (full calculation of cascades), and the random seed number.
- Line 6 is a comment
- Line 7 = Automatic disk datafiles of individual ion data (0=no, 1=yes).
- Line 8 is a comment
- Line 9 = Target description (in quotes), number of elements and number of layers in target.
- Line 10 is a comment
- Line 11 = Plot display type for ion animation during calculation; Viewing window (Angstroms) for calculation (this window defines the 100 bins for the average ion collisional data; 0 0= show entire target).

- Line 14 is a comment
- Line 15+ = (first 14 characters are ignored) then target element atomic number and weight (amu). Target elements are listed until they reach the total number of elements in target as specified in Line 9. Then two lines of comments about target, then the target data: Layer number, Layer description (in quotes), Layer width (Å), Layer density (g/cm³), Stoichiometry of each target element. After all target layers are complete, the final data line specifies the target as 0=Solid, or 1=Gas.

Note that after comment Line 14, *Target Elements: Z, Mass (amu)*, the number of data lines varies with the number of target elements and the number of target layers. TRIM expects that the number of these lines will conform with the data stated in line 9, *Number of Elements & Layers*. See next two examples of TRIM.IN for the format.

- Last 10 lines = Stopping corrections for special bonding in compound targets. Target energies (eV) for lattice binding, surface binding and displacement (one displacement energy for each target element). Finally, optional selection of stopping powers to be used in TRIM. See Ch.9.

Table 8-6 - Datafile TRIM.IN for DEMO: Xe(100 keV) into Si/Pt/Si.

```
==> SRIM-2008.01 This file controls TRIM Calculations.
Ion: Z1 , M1,  Energy (keV), Angle,Number,Bragg Corr,AutoSave Number.
    54    131     100       0  999999      0     10000
Cascades(1=No;2=Full;3=Sputt;4-5=Ions;6-7=Neutrons), Random Number Seed, Reminders
                        2                   0             0
Diskfiles (0=no,1=yes): Ranges, Backscatt, Transmit, Sputtered,
          Collisions(1=Ion;2=Ion+Recoils), Special EXYZ.txt file
                      0     0     0     0     0
Target material : Number of Elements & Layers
"Xe into Si/Pt/Si [Mixing a Marker]"   3    3
PlotType(0-5);Plot Depths: Xmin, Xmax(Ang.)
     0              0      300
Target Elements:    Z    Mass(amu)
Atom 1 = Si =       14      28
Atom 2 = Pt =       78     195
Atom 3 = Si =       14      28
Layer   Layer Name  Width Density  Si(14)  Pt(78)  Si(14)
Numb.  Description  (Ang) (g/cm3) Stoich  Stoich  Stoich
 1    "Silicon"    200    2.33     1       0       0
 2    "Platinum"    30   21.4      0       1       0
 3    "Silicon"     70    2.33     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       21
Individual target atom lattice binding energies (eV)
    2.1     2.2     2.1
Individual target atom surface binding energies (eV)
    3.1     3.2     3.1
Stopping Power Version (1=2008, 0=2003)
 1
```

The description of this TRIM.IN file is the same as the previous one, except that it has two different elements in the target with three layers. Note that there is a further explanation of TRIM.IN in Chapter 9, which contains more details.

Table 8-7 - **Datafile TRIM.IN for Demo: H(50 MeV) into Biological Target**

```
------------------ Input Data File for TRIM ----------------
Ion:Z1,M1, Energy (keV), Angle, Number, Bragg Corr, AutoSave Number.
    1 1.01      50000         00.0   99999     0.00             500
Cascades(1=No; 2=Full; 3=Sputt.; 4,5= Neutrons), Random Number Seed
                          1                              0
Diskfiles(0=no,1=yes) Ranges Backscatt Transmit Sputtered, Recoils
                       0        0        0         0        0
Target material :          Number of Elements & Layers
"H(50MeV) Irradiation of Thyroid"   12            5
Target Energies (eV): Binding, Surface, Individual Displacement
                  2.000  4.000 15 15 15 15 15 15 15 15 15 15 15 15
PlotType(0-5);Plot Depths: Xmin, Xmax(A) [=0 View Full Target]
              1            000000     000000
Target Elements:     Z      Mass (amu)
 Atom 1 =  H =       1     1.0080
 Atom 2 =  C =       6     12.011
 Atom 3 =  N =       7     14.007
 Atom 4 =  O =       8     15.999
 Atom 5 = Na =       11    22.990
 Atom 6 = Mg =       12    24.305
 Atom 7 =  P =       15    30.974
 Atom 8 =  S =       16    32.066
 Atom 9 = Cl =       17    35.453
 Atom10 =  K =       19    39.098
 Atom11 = Ca =       20    40.080
 Atom12 = Fe =       26    55.847
Layer Layer Name or Width  Density  H( 1)   C( 6)   N( 7)   O( 8)  Na(11)  Mg(12) P(15)
Numb. Description    (A)      (g/cm3)   Stoich  Stoich  Stoich  Stoich  Stoich
1   "Skin-Human #3"   12000.E+03  1.090E+00   0.62744 0.08237 0.01654 0.27202 0.00054
2   "Adipose Tissue"  40000.E+03  9.200E-01   0.63482 0.28408 0.00306 0.07775 0.00012
3   "Skel. Muscle #2" 60000.E+03  1.050E+00   0.63169 0.07432 0.01515 0.27703 0.00000.
4   "Thyroid (W&W)"   14000.E+04  1.050E+00   0.63870 0.06133 0.01061 0.28826 0.00054
5   "Skel. Muscle #1" 20000.E+03  1.050E+00   0.63169 0.07432 0.01515 0.27703 0.00000
0     Target is a SOLID
NOTE : Data for atoms S, Cl, K, Ca and Fe omitted in target description
above. Also, final 12 lines of TRIM.IN are omitted. See Table 8-6. For a full
TRIM.IN datafile, run the DEMO included in the TRIM Setup window.
```

This TRIM.IN shows a most complicated target, with twelve elements in five layers. This is a special input for biological targets. The target description shown is truncated at the right edge: the datafile actually continues to include the stoichiometry of S, Cl, K, Ca and Fe atoms. If you wish to make up a manual input file, like the above, first generate this file with the standard TRIM Input window and use the TRIM.IN file which is generated as a template.

Changing TRIM Plot Colors (TRIM.cfg)

All of the TRIM plots and colors are set using the datafile: **../Data/TRIM.cfg**, see Table 8-8. Typical default settings are shown in this Table. If you change a TRIM color, e.g. using the color tables available in the TRIM Calculation window, then when you save TRIM these changes become the default values.

Table 8-8 -Datafile ..Data/TRIM.cfg (TRIM Plot 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 plot of 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 TRIM.cfg. However, to change colors. 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 colors 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.

Changing The Maximum Size of Recoil Cascades (TRIM.cfg)

Using the datafile: **../Data/TRIM.cfg** (see Table 8-8) one can modify the maximum number of recoiling atoms in a detailed collision calculation. The default is 20,000, i.e. up to 20,000 recoils can be counted in a single recoil cascade. The ion may impact many atoms as it goes into the target. When it hits an atom and transfers a very large amount of energy, the recoiling atom may hit

thousands of other atoms before it stops. TRIM stores the data about each collision and each recoiling atom, until the prime recoil (the recoil that starts the cascade) is stopped. This storage of the kinetics of thousands of recoils takes a lot of computer memory, and so the default maximum is set at 20,000. However, this value can be increased. TRIM has been tested with a recoil cascade limit of 10,000,000 without any problems.

Incorporating SRIM into Other Software (SRIM Module)

"*SR Module.exe*" is a program that can run under the control of other programs that needs stopping powers and ranges. When it is executed, it reads a control file and then outputs a new file containing stopping powers and ranges. This output can then be used by the other programs. Since it has no user interface, it is invisible to the user.

SR-Module uses the same controls as the *"Tables of Stopping and Ranges"* which can be called from the SRIM Title Page. When *"Tables of Stopping and Ranges"* is run, the Setup program creates a file called "*SR.IN*" in the SRIM directory. It then calculates the requested stopping powers and ranges and places them in a separate file in the directory *"/SRIM Outputs".*

To use SR-Module, first look in the SRIM sub-directory *"../SR Module".* You will find a program "*SR Module.exe*", and data files: *SCOEF03.dat*, *SNUC03.dat* and *VERSION*. The first two are datafiles for the stopping and range program and the third contains the current version of SRIM.

You will also find a copy of the control file "*SR.IN*". It contains information such as:

Table 8-9 - File SR.IN controlling Stopping and Range Tables

```
1    Stopping/Range Input Data (Number-format: Period=Decimal Point)
2    ---Output File Name
3    "Hydrogen in Water_Liquid"
4    ---Ion(Z), Ion Mass(u)
5         1       1.008
6    ---Target Data: (Solid=0,Gas=1), Density(g/cm3), Compound Corr.
7                     0                    1                 1
8    ---Number of Target Elements
9           2
10   ---Target Elements: (Z), Target name, Stoich, Target Mass(u)
11                       1   "Hydrogen"      2         1.008
12                       8  "Oxygen  "       1        15.999
13   ---Output Stopping Units (1-8)
14    5
15   ---Ion Energy : E-Min(keV), E-Max(keV)
16                   10          10000
```

SR Module reads this file and generates a file called "Hydrogen in Water_Liquid" containing the stopping and range of H ions into water from 10 keV to 10 MeV. The lines of the above file are explained below:

1   **Title line. Note that all numbers MUST use a period as a decimal point.**
2   **Comment describing the next input line.**
3   **Name of the Output File**
4   **Comment describing the next input line.**
5   **Ion Atomic Number and Mass**

6	Comment describing the next input line.
7	Target Data: [Target is a solid or gas], [Target Density- g/cm3], [Compound Correction]
8	Comment describing the next input line.
9	Number of target atoms (up to 100)
10	Comment describing the next input line.
11	Tgt Atom #1: Atomic Number, Name, Atomic Mass
12	Tgt Atom #2: Atomic Number, Name, Atomic Mass
13	Comment describing the next input line.
14	Output Stopping Units (1-8) [*see listing of units below*]
15	Comment describing the next input line.
16	Ion Energy Range, keV, of output tables (2 numbers)

To understand the details of this file, go to the SRIM program *"Tables of Stopping and Ranges"* and read the various HELP files. Execute this SRIM program to calculate a new Table, and then exit and look at the file *"SR.IN"*. You can copy this control file into the subdirectory *"../SR Module"* and then execute "*SR Module.exe*". You will find that it generates the same table, but with no input from the user. This new file will be saved into the current directory of *"SR Module.exe"*.

In the input file, the next to last item is "Output Stopping Units (1-8)":
> *(1) - eV / Angstrom*
> *(2) - keV / micron*
> *(3) - MeV / mm*
> *(4) - keV / (ug/cm2)*
> *(5) - MeV / (mg/cm2) = keV / (ug/cm2)*
> *(6) - keV / (mg/cm2) = eV / (ug/cm2) = MeV / (g/cm2)*
> *(7) - eV / (1E15 atoms/cm2)*
> *(8) - L.S.S. reduced units*

Use the SRIM program to generate several Tables, and look at each of the *"SR.IN"* files. These will guide you to make new control *SR.IN* files.

Using "SR Module" to generate customized tables of Stopping and Range.

When you produce the Tables, you specify the starting and final ion energy, but you do not control the spacing of the energy increments. However, you can generate stopping powers for any list of energies using "*SR Module.exe*" by using the following change to the above "*SR.IN*" file.

Line 15:	---Ion Energy : E-Min(keV), E-Max(keV)
Line 16:	0 0
Line 17:	1.02
Line 18:	2.55
Line 19:	3.98

Line 20:   **0**
(Additional Lines Omitted)

Line 16 used to contain the lowest and highest ion energies of SR.IN as shown in Table 8-9. Now it contains " **0   0** ". This indicates that the lines following this line will contain a list of specific energies. Enter your list of energies (up to 1000) and terminate the list with a " 0 " as shown above. The list shown above will generate a simple Output File that will look like:

> **Ion = Hydrogen   , Mass = 1.008**
> **Tgt = H + O (Solid), Density = 1 g/cm3**
> **Stopping Units = MeV/(mg/cm2)**
> **Energy(keV)   S(Elec)   S(Nuc)**
> **1.020E+00   1.751E-01   3.921E-02**
> **2.550E+00   2.694E-01   2.391E-02**
> **3.980E+00   3.264E-01   1.681E-02**

The top four lines of this output file allow a check of the input values. Then there is a list with three values on each line: [Energy (keV)], [Electronic Stopping Power], [Nuclear Stopping Power]. This file can then be read into another program which requires stopping powers for specific ion energies.

Calculation Individual Atom-Atom Nuclear Stopping Powers

The nuclear stopping powers of **SR Module** will be slightly different from those in the full tables since these are improved values which will be incorporated into SRIM. The Table **SNUC03.dat** contains individually calculated nuclear stopping powers for all possible combinations of ion/targets, i.e. it contains 92 x 92 individual nuclear stopping powers. The nuclear stopping used in SRIM is a scaled stopping power, often called "ZBL" in the literature. This approximation is quite good for the interaction of atoms of approximately the same mass. However, it is somewhat inaccurate for ion / target atoms with quite different masses, especially H or He ions. The values produced by the SR tables described above are quite good because they are specific for the ion/target atoms specified, and do not come from a "universal" formula.

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