. *Tutorial #2* – Target Mixing and Sputtering

The previous Tutorials has covered how to setup TRIM, determine which ion and energy to specify for a n-well implantation, and how to evaluate the damage during the implantation. This Tutorial will show other effects of ion/solid interactions.

. *Interface Mixing and Sputtering*

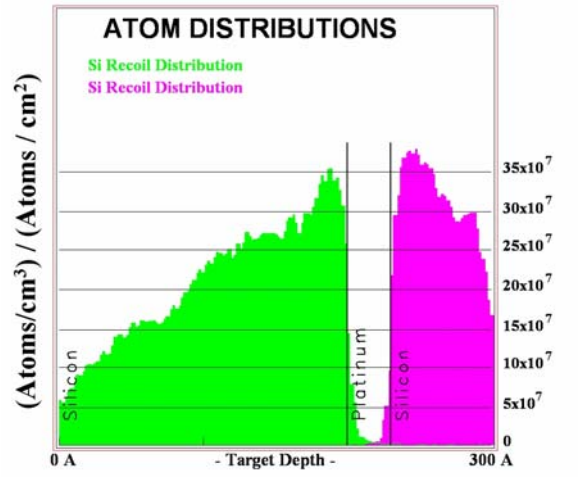
Interface Mixing is the transport of atoms from one layer of a target into another layer. This is usually an undesirable effect. We have seen how ions can transfer significant energy to recoil atoms, and these can move long distances and create significant collision cascades (see Tutorial #4). When a recoil atom crosses from one target layer to another, the second layer is contaminated.

However, there are special cases where recoil mixing is used to modify materials on purpose, and this process is called "**recoil implantation**". This technique is used for materials which are either difficult or dangerous to handle. An example is the fabrication of materials containing radioactive substances. For example, a thin layer of calcium may be deposited on a target of silicon, and then it is placed in a nuclear reactor to convert the calcium to a radioactive isotope. The silicon is then placed in an ion implanter, and a high dose of Xe ions are implanted into the calcium layer. The Xe atoms knock some of the radioactive material into the silicon, where it is trapped. After removing any remaining surface Ca, the silicon with implanted radioactive calcium can be safely handled. Such a target is useful to provide a sample which emits a radioactive particle (here from the Ca) but which is far less dangerous than a pure sample of radioactive Ca.

Sputtering is the opposite of Recoil Implantation. Here, surface atoms are removed from the target by creating recoil cascades that come back out of the target, and which give surface atoms enough energy so that they are driven away from the target. There is a binding force which holds atoms to the target, and this is called the ***Surface Binding Energy***, E_{surf}. An atom at the target surface is not confined on one side, so the energy required to remove it from its lattice site is less than if it was inside the solid and surrounded by other atoms. A surface atom has fewer electronic bonds which must to broken. E_{surf} is usually less that the Displacement Energy, $\mathbf{E_{disp}}$, for the solid.

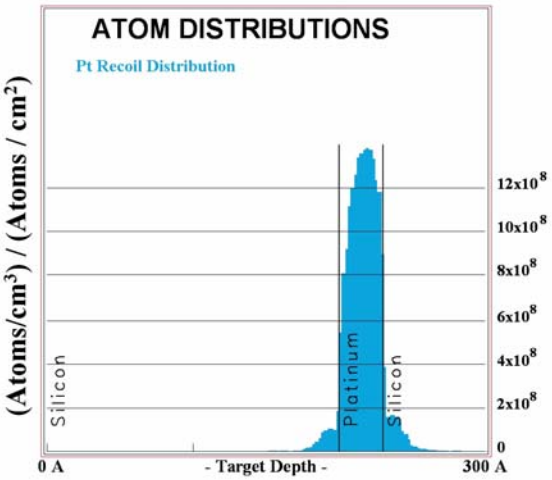
- Open SRIM by clicking on its icon on your desktop.
- In the window, click on **TRIM Calculation** to open the TRIM Setup window.
- Press **TRIM DEMO**. This window will generate the input for 12 examples which show how TRIM can be used for different applications. Press the button for: **Xe into Si/Pt/Si (Mixing a Marker)**. Look at the various inputs to the TRIM calculation. Then press Save Input ant Run TRIM. The window will close, and TRIM will immediately start.

. *Target Mixing*



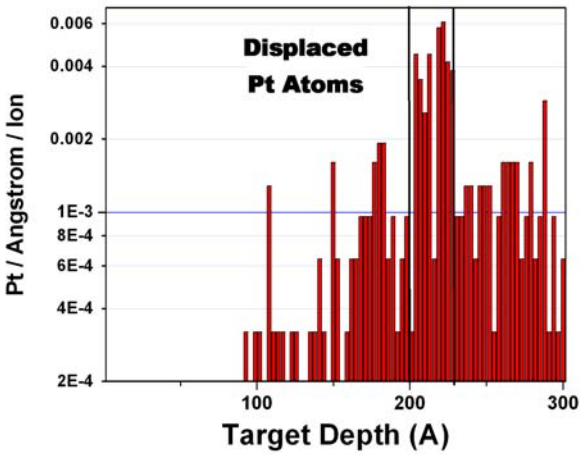
This example shows a thin Pt layer, inside a target of silicon. It was chosen to show how large the effects of interface mixing might become.

Click on the plot: ***Ion/Recoil Distribution***. In the sub-menu that appears, select "***2 – Silicon Recoil Distribution"*** and "***4 – Silicon Recoil Distribution"*** and then ***Plot***. The two silicon recoil distributions will be in different colors to separate the two contributions. After just a few ions, less than 100, the gap holding the platinum layer will start filling up with silicon atoms. By 400 atoms, this layer will be almost 5% silicon. The transfer of atoms into this layer is very efficient for a heavy ion such as Xe (atomic number = 54). Close this plot window.



Again, click on the plot: ***Ion/Recoil Distribution***. In the sub-menu that appears, select ***3 – Platinum Recoil Distribution***, and then ***Plot.*** This plot shows the platinum layer atoms, and how many have moved into the silicon. Of particular note is that the number of platinum atoms displaced towards the surface is quite large, at least 50% as large as the platinum atoms driven deeper into the target. This is remarkable! The ions are flying deep into the target, and all the initial recoils are generally starting in the same direction, i.e. deeper into the target. How can atoms end up at a shallower position than where they start?

To see the answer, click on the ***XY Longitudinal*** plot that shows each ion and the displacements that it causes (This plot button is in the section ***Collision Plots***). At the bottom of this plot is a button marked **Clear**. This will clear the plot so that you can see individual ions and the recoil cascades that are generated. The ion track is a thin line of red dots, where all recoil cascades must start. Each recoil cascade (not the ion's cascades) begins in a forward direction, but rapidly spreads out into almost random directions. The dense cascades look like balls of green dots, with no special direction. The cascades involve so many particles that any "knowledge" of the original ion direction is rapidly lost. The cascade becomes an isotropic event, i. e. the atoms go in every direction. (Note: for high performance PCs, it may be necessary to press "***Clear***" and then press "***Pause***" at the top of the TRIM window. This will stop the display after the next ion.)



This is what causes backward moving Pt atoms, which move towards the target

surface. The big cascades rapidly lose any forward direction and become isotropic. The degree that this happens is indicated by the difference in the number of Pt atoms which are forward scattered, deeper into the silicon, and the number scattered back towards the target surface.

A second feature to note is the large distance that the platinum atoms will move. The original Pt layer is 30 Angstrom thick. Within 500 incident ions, you will begin to see platinum atoms driven more than 30 A from the Pt layer.

If you go to the TRIM DISTRIBUTIONS box and press the ***File*** button command for ***Ion/Recoil Distributions***, you will get a numerical table which shows more details than the plot. This file is placed in the SRIM folder: „/***SRIM Outputs***, and it is called ***RANGE.txt***. It shows that some Pt atoms have recoiled far back from the Pt layer – within 100 Å of the surface, and others have reached the back edge of the target. The recoil mechanism is so efficient that Pt atoms are driven throughout the silicon target with fewer than 500 incident ions. If TRIM is continued for several thousand ions, some of the Pt atoms will be found to have moved back through the target surface, and are lost from the target.

Let the above TRIM calculation continue until more than 1000 ions are completed. You can increase the speed of calculation by closing all plot windows, which slow down the calculation.

. *Target 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.

Sputtering Yield = (Number of Sputtered Atoms) / (Number of Incident Ions)

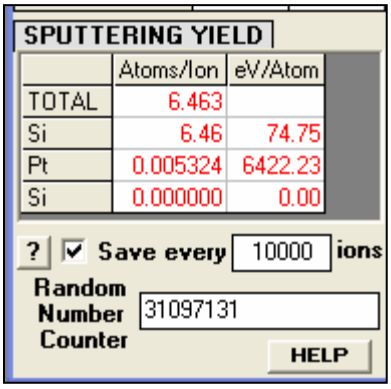
The surface binding energy (SBE) of an atom to a surface is known only for a few materials, but it is common to use the ***heat of sublimation*** as an estimate. Typical values are: Ni (4.46 eV), Cu (3.52 eV), Pd (3.91 eV), Ag (2.97 eV), Pt (5.86 eV) and Au (3.80 eV). Values will be suggested when you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

. *Comments on Sputtering*

- Only the cascades which come 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 300 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 1000 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 at which target depth the sputtering yield remains constant.

- 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 energy changes under bombardment due to surface roughness and damage, and also due to changes in the surface stoichiometry for compounds. The sensitivity of sputtering yield to surface binding energy may be displayed during the calculation by using the plotting menu. The plots of sputtering yield to SBE are accurate to about 30%.

[For cascades within the target at very low energy (which is a major contributor to sputtering) TRIM uses 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.]

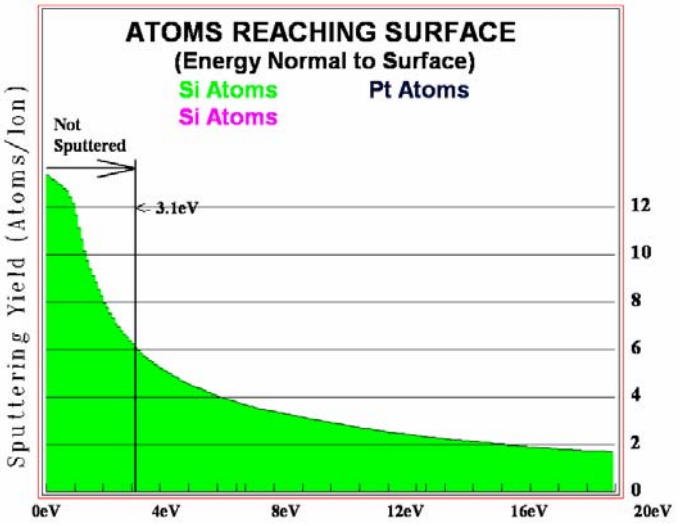


It is possible that some of the recoil cascade atoms which exit the target have originated from deeper inside the target than just the surface. We will see that some Pt atoms are seen to sputter from collisions that begin more than 200 Angstroms inside the target.

Now look at the right side of the TRIM window at the section called **SPUTTERING YIELD (SY)**. This gives the number of atoms which have been sputtered per incident ion. You will see that ~ 6 or 7 silicon atoms are sputtered for each incident ion. The ions are actually digging a hole, for more atoms are leaving than arriving, by 6 to 1! Further, if you have run at least 1000 ions, you will see that there is even a number of platinum ions which have sputtered. The Pt sputtering yield is shown as =.005324 (about 1 every 200 ions). They started 200 Angstroms inside the target, and some of the cascades have been so energetic that the platinum atoms were transported back through the top surface!

- Pause the TRIM calculation by pressing **PAUSE** at the top of the TRIM window.
- At the left, under **DISTRIBUTIONS**, press the plots: **Integral** and **Differential Sputtered Atoms**

Look first at the plot called ***Sputtering (Integral)***. The plot name is shown at the top of the plot window. This plot shows the energy of every recoiling atom which reaches the target surface. The ordinate has units of ***Atoms/Ion***, so each ion will produce about this number of recoiling atoms which reach the surface. There is a vertical bar marked ***3.1 eV***, which is the average **Surface Binding Energy, E_{surf},** which was entered for silicon in this target. To the left of this bar is an arrow with the legend ***Not Sputtered***. At 3.1 eV, the number of atoms which reached the surface with more than this energy is about 7. This is the number of atoms sputtered, and it agrees with the number we saw in the **SPUTTERING YIELD** table above.



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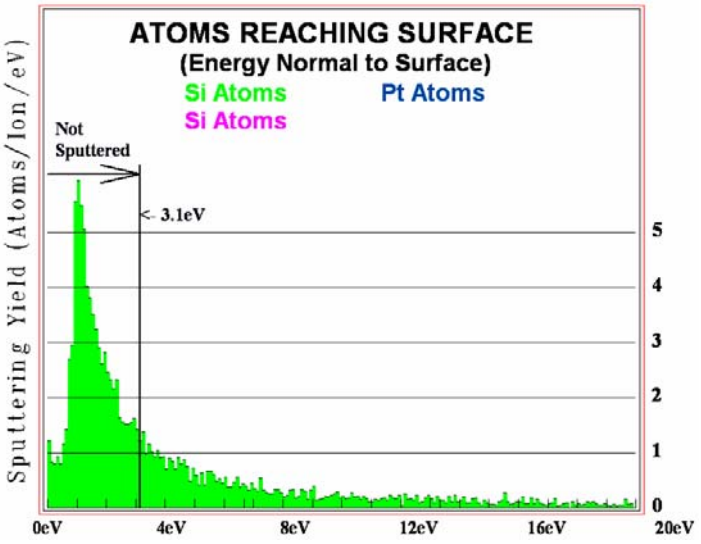
One comment should be made about the Surface Binding Energy. This is the minimum energy which an atom must have to be sputtered. It should be clear that only the *normal component* of the ion's energy should be counted. That is, an ion which reaches the surface with a trajectory of 45^o to the surface, will actually need 1.4 x E_{surf} to be sputtered. In the plots that you will create below, this correction is automatically included. The atom energies shown are always the normal component the atom's energy, not its total energy.

The value of the Surface Binding Energy probably changes with irradiation. This is because the sputtering of a target makes it rough and damaged, and rough targets tend to have reduced Surface Binding Energies. As the target roughens, the sputtering yield will go up as each surface atom is tethered to the surface by fewer electrons. Hence the calculation of sputtering does not include all effects – especially a surface binding energy that changes with time as the beam roughens the surface. But this plot allows us to estimate how much this Sputtering Yield might change with time. We can see that if the Surface Binding Energy would be reduced in half, the sputtering would increase less than 2x. And even if the Surface Binding Energy would be reduced to ZERO, the sputtering yield would increase only by 2x. **So the calculation will be accurate within 2x, no matter what happens to the target surface.**



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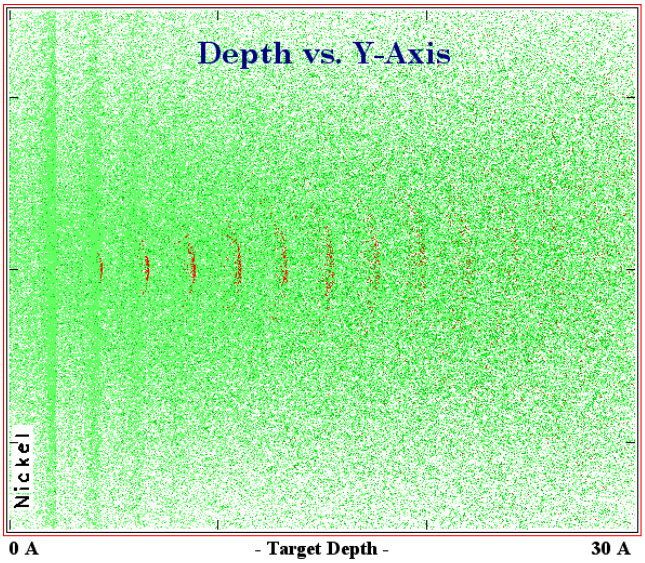
Click on the plot **SPUTTERING (Differential)** to bring it to the top. This plot is the differential of the previous Integral plot. The Integral Plot shows the number of atoms reaching the surface with a given energy of more. This plot shows the distribution of atom energies reaching the surface. The most common energy is very low, about 1 to 2 eV.

Stop the TRIM calculation. You can do this either by pressing the windows Close box **X** in the upper right of the window, or by pressing **File** and ***Exit***. When asked if you want to SAVE the calculation, press **NO**. The TRIM calculation window will close, and you will return to the TRIM setup window.

- Try a different calculation by pressing **TRIM DEMO** and then select ***Sputtering: Xe into Nickel***. This calculation will show an extreme example of sputtering.

As the calculation proceeds, in the starting plot called ***XZ Longitudinal***, you will see that the red dots showing displacements by the ion begin to cluster in vertical lines. The spacing between atoms in Nickel is slightly more than 2 Angstroms, and this is the separation between the groups of crescent red dots. The incident ion can only have one collision for each monolayer of target, so when you look at this plot (the total target width is less than 15 atoms) you can see actual atomic structure. After a period of time, the green dots will also begin to show the same striations. Again, this is due to the atomic spacing of the target.



Press the DISTRIBUTIONS plot: ***Integral Sputtering***. This plot indicates that more than 10 atoms are sputtered for each incident ion. But the slope of the integral of atom energies is much steeper than for the previous silicon target. If the surface roughens, and the Surface Binding Energy of the target is reduced, the sputtering yield may go up 2x or even 3x. Hence for this case, the sputtering calculation is only a rough estimate because we can not predict the surface roughening. Such roughening depends, for example, on the grain size of the poly-crystalline nickel. This effect can not be incorporated into TRIM.

Detailed data about all sputtered atoms can be recorded by pressing the File button. This creates a file called "SRIM Outputs\SPUTTER.txt". A typical example of this file is shown below. (Note that this file must be formatted using the font MS-LineDraw to get the various lines and boxes in the report.)

. *SUMMARY : Mixing and Sputtering Calculation:*

- ***Interface Mixing can be a large effect with atoms moving more than 100A from initial position.***
- ***Significant number of atoms move towards the surface. These also can move long distances.***

- ***Sputtering can rapidly erode the surface with more than 5 atoms leaving for each incident ion.***
- ***Some atoms which sputter come from deep in the target, as seen for the Pt atoms which sputter from more than 200 Angstroms below the surface.***

. *Example of datafile SPUTTER.txt*

```
    ========================================================================
                          SPUTTERING   CALCULATION
    ========================================================================
    =   AXIS DEFINITIONS: X=Depth, Y,Z= Lateral plane of target surface.=
    =   Shown are: Ion Number                                            =
    =              Sputtered atom type (atomic name) and energy (eV)     =
    =                 (Note: SBE is NOT subtracted from atom energy)     =
    =              Point of ejection relative to ion entrance point.     =
    =              Trajectional cosines of ejected atom.                 =
    =                  Cosine (X) is negative indicating motion away     =
    =                     from the target surface.                       =
    =                  Cosine (Y) and Cosine (Z) are transverse motion.  =
    ========================================================================
     ================== CALCULATION   DATA  ============================
```

Xe(1 keV) ==> Si(100 A)

Ion Numb	Atom Numb	Energy (eV)	Depth X(A)	Lateral-Position Y(A)	Lateral-Position Z(A)	Atom Direction Cos(X)	Atom Direction Cos(Y)	Atom Direction Cos(Z)
1	1	2219	00E+00	-.397E+01	.174E+02	-.73966	-.45399	.49676
1	1	2281	00E+00	-.391E+01	.143E+02	-.56877	-.43337	-.69906
1	1	222	00E+00	-.758E+01	.161E+02	-.92030	.02871	.39015
1	1	223	00E+00	-.835E+01	.152E+02	-.39997	.77688	.48627