. *Tutorial #4* - Calculations of Target Damage

SRIM Tutorial #1 showed how to construct a CMOS n-well in silicon that would give a peak concentration of n-type dopants of about ~$5x10^{18}$ atoms/cm^3, with the peak depth being 250 nm. The question was to select the correct dopant, and to find the implantation energy and dose (ions/cm^2) to achieve this n-well structure. The Tutorial ended with the selection of phosphorus ions at 190 keV, with an implant dose of about 10^{14} ions/cm2

This tutorial will expand on the complicated subject of target damage by ions, and will use the target of Tutorial #1 for this discussion.

Normally, implanting at room-temperature, 300^{o}K, will cause most of the implantation damage to "self-anneal". The target damage disappears because at room temperature, the lattice atoms have adequate energy to allow simple target damage to regrow back into its original crystalline form. In general, metals self-anneal faster, and insulators slower than the semi-conductor silicon, so a silicon target makes a good example. However, there are no thermal effects in SRIM, so the damage which is calculated is that which would happen for an implantation at 0^o K. Ignoring thermal effects changes the quantity of final damage, but the basic damage types which are discussed will still occur.

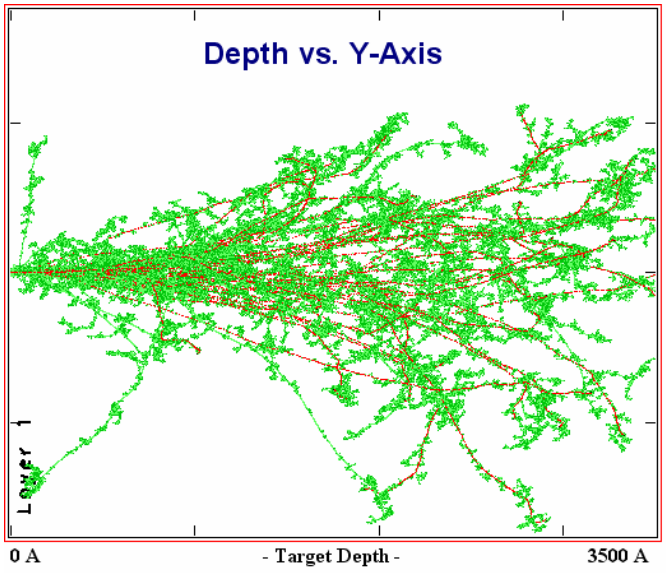
First, set up the same calculation in SRIM as was used in Lesson #1 :

- Click on the SRIM icon on your desktop.
- In the opening window, click on **TRIM Calculation**.
- Go to ION DATA and click on **PT** button. Select **Phosphorus**.
- On this same ION DATA line, in the box: "***Energy (keV)"*** you need to enter **190.**
- Go down to TARGET DATA. Find the **PT** button for the target. Select **Silicon**.
- Go to the LEFT side of this line, and for "***Width***" enter **3500 Ang.**
- Go to the LEFT side of this line, and for "***Layer Name***" enter "**Silicon**" (instead of *"Layer 1")*
- Go to the TOP-RIGHT box "DAMAGE". Scroll down to select "***Detailed Calculation with Full Damage Cascades***".
- The setup is complete. Look at all the boxes to check that you have entered the right numbers. Also look at some of the other entries. Press the Help button, **?** , for each item to obtain full explanations of that entry.
- Finally, press **Save Input and Run TRIM**

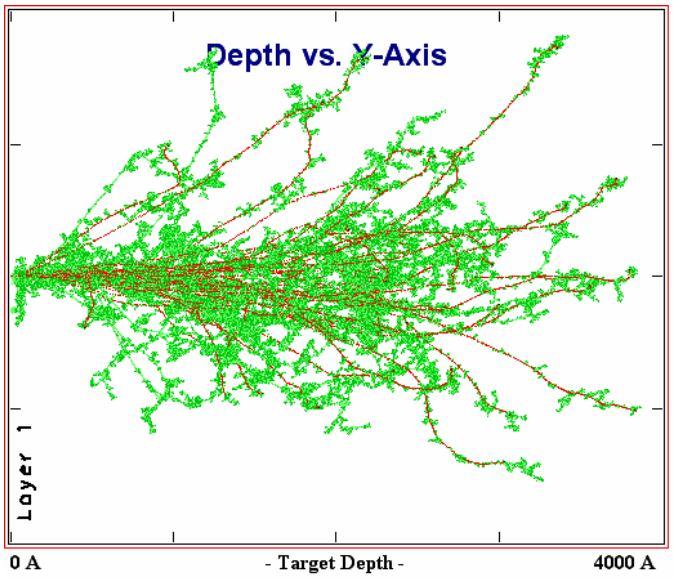
TRIM opens and the calculation immediately begins.

There is a plot in the center that shows the calculation results for each ion. The red dots are those collisions between the ion and target atoms in which the target atoms are knocked from their lattice sites. The green dots are collisions between recoiling target atoms, silicon, and other target atoms. The recoiling target atoms cause collision cascades which dominate the damage process. The dot is only plotted if the transferred energy is large enough to displace the atom hit from its lattice site. Thus the plot shows the number of displacements which have occurred. There is a different color used to show where each ion stops, but this single black pixel is so small on modern high-resolution screens that it is hard to see.

Note the upper left "ION" box, which repeats the Ion data. Note the "TARGET DATA" window, which contains all target information (you may have to expand this window with your cursor). Some of this information you did not enter, such as Displacement Energy (15eV), Surface Binding Energy (4.7eV), and Lattice Binding Energy (2eV). The values given are the default values for silicon. These will be explained later in this lesson.



First, we will play with some TRIM controls so that you can understand its flexibility. Pause the calculation by pressing **Pause**. Now press **Change TRIM**. This will allow you to change the input values to modify the calculation. For example, let's change the color of the recoiling silicon atoms from green to blue. *(Note that the colors mentioned may differ on your PC if someone has previously altered the default colors for SRIM)*. Click on the colored square labeled "***Moving Atom Colors"***. A palette of colors will appear. Pick a blue. Press **OK**. Press **End Edit**. Press **Continue**. The new recoiling silicon atoms will be colored blue when they make a vacancy. This blue dots are overwhelmed by the green silicon "stopping atom" dots, but you should see a few in the collision cascades.



Notice in the plot of the ion tracks, that some of the ions appear to be leaving the target to the right. The target is not deep enough to capture all the ions. To correct this, pause the calculation by pressing **Pause**. Now press **Change TRIM**. Click in the *Target Data* window: ***Width (A)*** **3500**. A popup menu will appear so that you can change this target depth to 4000. You will also need to change the **Plot Window** displayed on the left in the *Plots* window. This should also be changed to 4000 so that you will be looking at the full target depth. After making this change, press **End Edit**. Press **Continue**. Since we are making a fundamental change in TRIM, the calculation restarts from the beginning. The plot has changed so that it is now showing a depth of 0-4000Å. And the ions are now all stopping before they go off the plot.

The purpose of this exercise was to show that you don't need to know all the variables to start TRIM. Perhaps you are unsure about what is the maximum depth of the furthest ion. You can start TRIM with approximate values, and then change them to more suitable values after you see what happens.

Let the TRIM calculation continue while you read the next two pages of explanation.

. *Scientific Background – "The Physics of Recoil Cascades"*

This section discusses terms used in evaluating the damage caused by energetic ions to a solid target. We need first to define basic terms.

The various parts of target damage are defined as:

- ***Displacement*** = The process where an energetic incident atom knocks a lattice atom off its site.
- ***Vacancy*** = A empty lattice site (without an atom). Originally all lattice sites are occupied, and displacements cause vacancies.
- ***Interstitial Atoms*** = Atoms which were knocked out of their original site, and come to a stop in the solid. Also the incident ions, when they stop, are considered interstitial atoms.
- ***Replacement Collisions*** = Atom sites with new atoms, identical to their original atom (this is discussed below). This is the only mechanism in which a vacancy may be re-occupied.
- E_{disp} = ***Displacement Energy***, the minimum energy required to knock a target atom far enough away from its lattice site so that it will not immediately return. This minimum energy produces a "*Frenkel Pair*" = a single vacancy and a nearby interstitial atom, which is the most fundamental type of damage caused by an ion.
- E_{latt} = ***Lattice Binding Energy***, the minimum energy needed to remove an atom from a lattice site. It takes energy to break electronic bonds and displace an atom from a lattice site, so this part of the energy transferred to a recoiling atom is lost. The lattice binding energy must be smaller than the Displacement Energy.
- E_{surf} = ***Surface Binding Energy.*** 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. This energy is especially important for calculating sputtering (removal of surface atoms).
- E_{final} = ***Final Energy of a moving atom***, below which it is considered to be stopped. The calculation of ion kinetics has to end at some minimum energy. The various energy loss processes tend to become smaller as an ion slows down, and a minimum energy creates a more efficient calculation. The Final Energy is an energy below any of the above energies.

For silicon targets, the default values are: $\mathbf{E_{disp}}$ = 15eV, $\mathbf{E_{latt}}$ = 2eV, $\mathbf{E_{surf}}$ = 4.7eV and $\mathbf{E_{final}}$ = 2 eV.

If a moving atom hits a target atom, and it transfers more than E_{disp}, the target atom will be ejected from its lattice site. Its recoiling energy, $E_{recoil} = E_{disp} - E_{latt}$, since it will lose E_{latt} energy to the lattice. The target recoil atom, if its energy is greater than E_{disp}, may go on and create further vacancies by hitting other target atoms.

There is special damage type that must be considered. If the incident atom is the same element as the atom that it hits, then the incident atom might transfer is energy to the target atom, knock it out of its lattice site, and the incident atom will then take its place in the lattice, while the hit atom moves on. This is called a ***Replacement Collision.*** Although this may sound complicated, this mechanism may reduce the total vacancies by up to 30%. ***Three different elements must be met for a Replacement Collision***.

(1) The moving atom must be identical to the target atom.

(2) The incident atom must end with less energy than E_{final} (it must stop).

(3) The struck atom must have enough energy to move on, i.e. its energy is greater than $\mathbf{E_{disp}}$.

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.
- An ***Atomic Displacement*** occurs if $E_2>E_{disp}$ (the hit atom is given enough energy to leave the site). A ***vacancy*** occurs if both $E_1>E_{disp}$ and $E_2>E_{disp}$ (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_{latt} before it has another collision. If $E_2<E_{disp}$, then the struck atom does not have enough energy and it will vibrate back to its original site releasing E_2 as ***phonons*** (energy deposited into crystal lattice vibrations).
- After a collision, if $E_1<E_{disp}$ and $E_2>E_{disp}$ 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 $E_1<E_{disp}$ and $E_2>E_{disp}$ and $Z_1 \neq Z_2$, then Z_1 becomes a stopped ***interstitial*** atom.
- Finally, if $E_1<E_{disp}$ and $E_2<E_{disp}$, then Z_1 becomes an ***interstitial*** and E_1+E_2 is released as ***phonons***. If your target has several different elements in it, and each has a different displacement energy, then E_{disp} will change as each atom of the cascade hits different target atoms.

These sum of these damage types are related. If you understand these two equations, then you have a good grasp of the above definitions.

Displacements = Vacancies + Replacement Collisions ***(Eq. 1)***
Vacancies + Replacements = Interstitials + (Atoms which leave the target volume) ***(Eq. 2)***

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 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 a recoil atom leaves the target, clearly the sum of interstitials will be less than the number of vacancies by the loss of that atom. Each replacement collision reduces the number of vacancies and the number of interstitials by one, leaving Eq. (1) in balance.

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. This topic is covered in the TRIM textbook, see Chapter 7 “The Scientific Background of TRIM”.
The following references can be used for background:

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).

Questions- See if you can answer the below questions without looking back. Then check your answers. (Answers at the end of this Tutorial)

(1) Does every displacement of a target atom lead to an interstitial ?

(2) What is the difference between the Lattice Binding Energy and the Surface Binding Energy of a target atom?

(3) If you implant silicon ions into a silicon target, can the incident silicon ion become a "Replacement Collision"? Why?

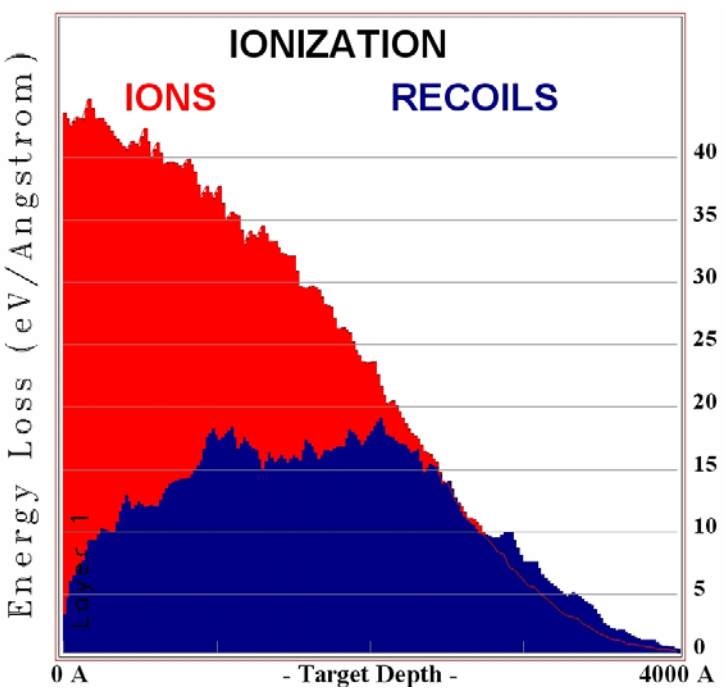
. *Energy Loss to Ionization and Phonons*

We will now look at two simple plots: ***Ionization*** and ***Phonons***.

Ionization is energy loss to the target electrons. The electrons of the target absorb energy from the fast moving ions and recoil atoms, and then release it as heat if the target is a metal, or as phonons if the target is an insulator. The plot shows ionization from the incident ions and also from recoiling target atoms.

Phonons are energy stored in atomic vibrations in a crystal. Since all the atoms in a crystal are linked, when you start vibrating one of them, then many of the other atoms start vibrating. This mass vibration is described as a phonon, since it is somewhat quantized (certain vibration modes are preferred).

We are assuming that TRIM has been running while you have been reading all of the above definitions and explanations.



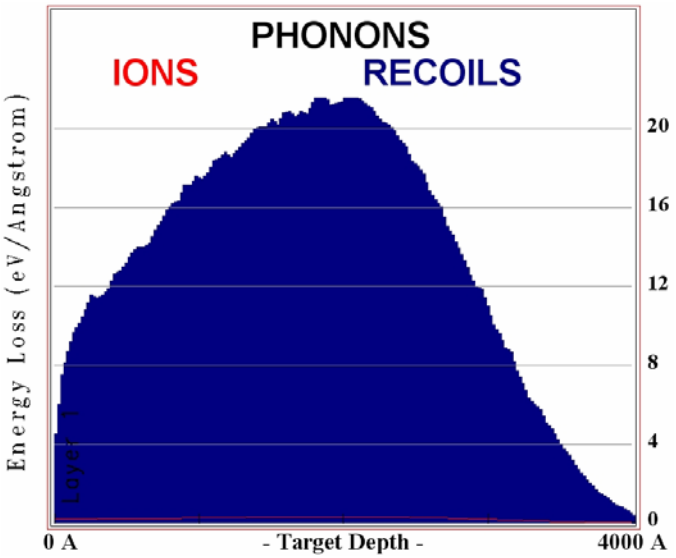
Open the ***Ionization*** plot by clicking on its box in the *Plot* window. (See plot on previous page.) There are two distinct plots, one for electronic energy loss from the incident ions, and one for energy loss from recoiling target atoms. In general, the ions have more ionization energy loss, but this is not true for all ion/target combination. The electrons tend to absorb energy most efficiently from particles whose velocity is similar to their velocity. The ions are moving much faster than the recoiling silicon target atoms, so the ions lose more energy to the target electrons.

Close the ***Ionization*** plot, and open the ***Phonon*** plot.

This plot shows the energy loss to phonons to be very different than that for Ionization. You can barely see the energy loss to phonons from the ions (red line at the bottom of the plot), and the phonons are produced almost exclusively by the recoiling target atoms. Where do these recoil-phonons come from? We don't know quite yet (it will be explained by another plot), but you can look at the window called *Calculation Parameters* on the right. The section called **"% Energy Loss**" shows how the incident energy of each ion (190 keV) is dissipated. The row called ***Phonons*** shows that the Ions are losing only a small amount of their energy, ~0.44%, to phonons (190 keV x 0.44% = 836 eV), while the Recoils are depositing ~30% of the energy into phonons (190 keV x 29% = 55 keV).

How are phonons made?

The phonons come from several sources. When an atom is knocked out of its lattice site, its binding energy, E_{latt}= 2 eV, is deposited into phonons produced by the recoils. If you look at the upper right box in TRIM, you will see how many vacancies are produced by each ion, Vacancies/Ion = ~ 2300. So for each ion, displacements by the ion or recoil cascades cause 2300 x 2 eV = 4,600 eV of phonons.



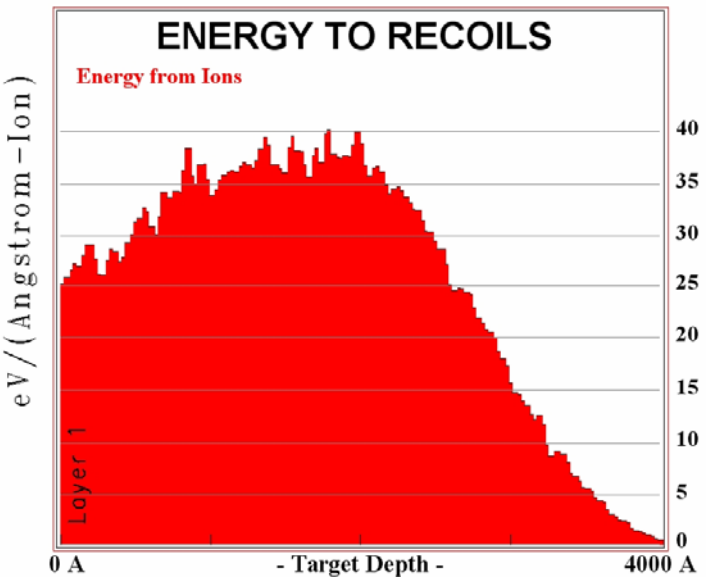
- The rest of the phonons are caused by either the ion or a recoil hitting a lattice atom and transferring less than E_{disp} of energy. At least E_{disp} must be transferred to a target atom to eject it from its site. What happens if less than this energy is transferred? Then the target atom recoils and vibrates for a while, but it doesn't have enough energy to bounce out of its site, and the energy is finally given to new phonons.

- The TRIM box on the right called "**% Energy Loss**" allows you to divide the incident ion energy into various types, including phonons. The ions generate phonons with 0.44% of their incident energy of 190 keV, and the recoiling atoms contribute an additional 28.8% = 29.2% (total). Multiplying by the total ion energy, 190 keV x 29.2% = 55 keV of phonons per incident ion. Assuming phonons add directly to target temperature, this can make the target quite hot. ***Close the Phonon Plot***.

% ENERGY LOSS	Ions	Recoils
Ionization	44.31	23.77
Vacancies	0.13	2.51
Phonons	0.44	28.85

. *Damage Creation in the Target*

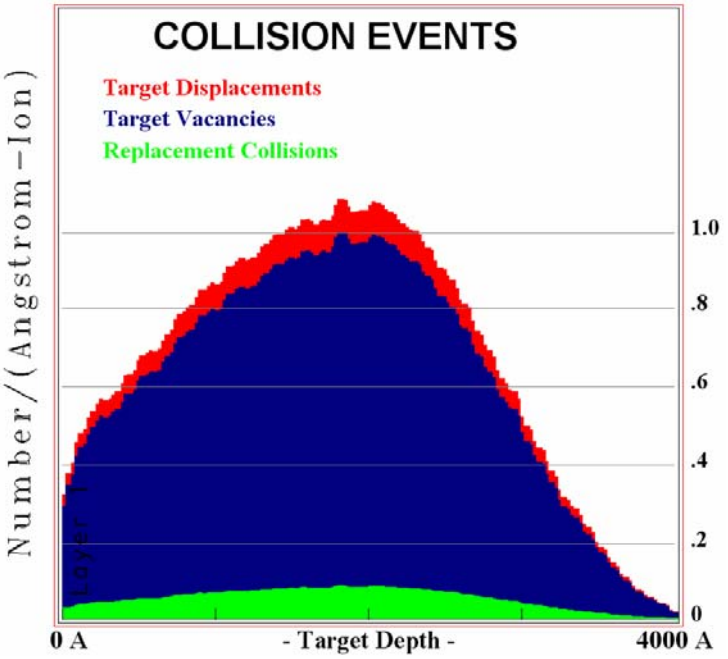
The next two available plots will show how the target damage is being created. In the *Plot* window, click the plot box: ***Energy to Recoils***. A box will open asking whether you want to plot ***Energy from Ions***, or ***Energy absorbed by Silicon atoms***. You can pick either one. This selection is important if there are more than one element in the target, and you want to find out how much each type absorbed. For our simple case, there is only one plot because all the energy deposited by the ions will be absorbed by silicon atoms. Both plots are identical for a single element target.



The energy transferred to target atoms is

fairly constant down to the mean range of the ions, ~ 2500 Å, and then it falls off as the ions stop. Other ion/target combinations may be quite different.

How much energy is transferred to the recoil cascades? Looking at the "***% Energy Loss***" box again, we can add up the energy deposited by the recoils: ~ 24%+3%+29% = 56% = 106 keV. So the ion deposits 44% of its energy directly to the target, and give up 56% to recoil cascades. Close the ***Energy to Recoils*** plot.



Open the plot: ***Damage Events***.

A menu pops up which contains all the damage details. Press the plots **#1** ***(Total Displacements)***, **#2** ***(Total Vacancies)***, and **#3** ***(Replacement Collisions).*** Then press :

Show Plot Numbers 1 2 3.

The higher curve shows the **Total Target Displacements**. This is the number of atoms knocked off their target lattice site. The next lower curve shows the **Target Vacancies**. This is lower than the Target Displacements curve, showing that there are fewer vacancies than displacements.

Why are there fewer vacancies than displacements?

The lowest curve shows the ***Replacement Collisions***. These are displacements in which the incident atom gives up almost all of its energy, and it does not have enough to continue further, and it falls into the vacancy left by the recoiling target atom. That is, it knocks out a target atom, and then replaces it in the lattice. Since it is the same element, there is no change in the target. As you can see, *the sum of the lower two curves equals the upper curve of Displacements*. Remember the equation shown in the ***Physics of Recoil Cascades*** section:

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

In this case, almost 10% of the displaced atoms do not leave vacancies, but instead are replaced by another silicon atom.

Are Replacement Collisions a significant portion of the target displacements?

How much do they reduce target damage in this example?

Answers to Questions in this Tutorial:

Remember the two basic equations of target damage:

Displacements = Vacancies + Replacement Collisions ***(Eq. 1)***
Vacancies + Replacements = Interstitials + (Atoms which leave the target volume) ***(Eq. 2)***

(1) Does every displacement of a target atom lead to an interstitial ?

No. When we combine Eq. (1) and (2) we can obtain:

Displacements = Interstitials + (Atoms which leave the target volume)

As long as the collision cascades remain within the target volume, then every displacement will yield an interstitial. If recoiling atoms leave the target, then they are not counted as interstitials. The total number of interstitials may be increased if you also count the incident ions that end within the target, but this is an exception to the general rule counting the displaced atoms minus any atoms that leave the target volume.

(2) What is the difference between the Lattice Binding Energy and the Surface Binding Energy of a target atom?

Lattice Binding Energy is the minimum energy needed to remove an atom from a lattice site. It takes energy to break electronic bonds and displace an atom from a lattice site.

Surface Binding Energy. 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, so it is usually considered to be less than the Lattice Binding Energy.

(3) If you implant silicon ions into a silicon target, can the incident silicon ion become a "Replacement Collision"? Why?

Yes. Although normally one defines *Replacement Collision* as a recoiling target atom knocking out another target atom of the same element, and replacing it in the lattice. Hence it replaces the atom since it is the same element, there is no change in the target lattice site. However, if your ion is the same element as one of the target atoms, it can also knock out one of these atoms and replace it. But this is not a common occurrence, and usually one expands the definition of *Replacement Collision* to include these rarer events.