. Tutorial #1- Introduction to Ion Ranges, Doses and Damage

This Tutorial will cover how to find the energy and dose of ions required to implant atoms into a target at a given depth and concentration. To illustrate this, we will assume that we wish to implant the n-well of a CMOS semiconductor device. The implanted ions should be an n-type dopant (implanted atom) in silicon and have a peak concentration depth (***projected range***) of about 250 nm (2500Å) below the silicon surface. The peak dopant concentration should be $5x10^{18}$ atoms/cm^3. Although this seems complicated (especially if you are not an electrical engineer) it merely asks that ions of elements phosphorus (P) or arsenic (As) or antimony (Sb) be directed into a silicon target to a certain depth and concentration (atoms of P, As and Sb are all n-type dopants to silicon).

As an additional limitation, we will assume that your implanter (accelerator) is limited to 200 keV. [Note: TRIM sometimes uses Å units because this is about the width of a monolayer of atoms in a solid. 10Å = 1 nm. These units are common in assessing target microscopic damage.]

> **Questions :**
> - **Which element will your use?**
> - **What dose is required (ions/cm^2)?**
> - **Will your target be amorphous after the implant?**

This set of questions will be the subject of this Tutorial. By the end, you will be able to answer these questions for any ion into any target material.
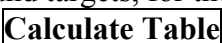
Finding Ion and Energy to Use

- Click on the **SRIM** icon on your desktop.
- Click on **Stopping and Range Tables** (S & R Tables)
  - First enter the ion. Start by clicking on the Help button ? next to "**ION**". Read the definitions and then close this window by pressing CLOSE .
  - In order to implant an n-well in silicon, you need to implant an impurity from column 5 of the Periodic Table. Typical dopants are Phosphorus (P), Arsenic (As) or Antimony (Sb). Start with the middle possibility: **Arsenic.** To enter an ion, use the PT button next to **Ion** in the window to bring up a chart of the elements. Select **As** as the ion.
  - The program will automatically fill in various boxes describing the ion. Note that this ion mass is not the average mass of arsenic, but the mass of the most abundant isotope, MAI. You can confirm this by activating the Periodic Table button, PT, which gives the various mass descriptions of arsenic.
  - Go down to **Target** in the window.. Click on this Help button, ? .
  - Specify target = **Silicon** using the PT button to specify **Si**.
  - Note that this target mass is not the MAI mass, but the average natural weight of the element. You can confirm this by activating the Periodic Table button, PT, which gives the various mass descriptions of silicon. Press Close to close the window.
  - The rest of the target table is blank, and not needed. The term "Stoich" is used for compound targets, for the stoichiometry of each of the elements of the compound.
  - Press **Calculate Table**.

- o Accept the suggested filename: "*SRIM Outputs\Arsenic in Silicon*". This file is stored in the SRIM directory: ***../SRIM Outputs/*** if you need to reference it again.
- Look at the table. What is the energy needed to have a ***Projected Range*** (depth of the peak concentration) of 2500Å? (Answer - *~400 keV*)

Ion Energy	dE/dx Elec.	dE/dx Nuclear	Proj. Range	Longit. Strag.	Lateral Strag
350.00 keV	1.876E+00	4.139E+00	2243 A	557 A	436 A
375.00 keV	1.944E+00	4.049E+00	2404 A	590 A	462 A
400.00 keV	2.013E+00	3.964E+00	2566 A	622 A	489 A
450.00 keV	2.150E+00	3.804E+00	2892 A	685 A	542 A
500.00 keV	2.285E+00	3.659E+00	3221 A	746 A	595 A

- Conclusion: This is a higher energy than your 200 keV implanter can reach!
- Redo the Range Tables but calculate using **Phosphorus (P)** ions.
- Look at the new table. What is the energy needed to have a Range of 250nm?

Ion Energy	dE/dx Elec.	dE/dx Nuclear	Proj. Range	Longit. Strag.	Lateral Strag
170.00 keV	1.789E+00	1.136E+00	2232 A	682 A	540 A
180.00 keV	1.833E+00	1.107E+00	2359 A	709 A	565 A
200.00 keV	1.914E+00	1.054E+00	2612 A	761 A	615 A
225.00 keV	2.008E+00	9.960E-01	2928 A	823 A	674 A

- This table shows that we can implant the n-well with a peak at 2500Å (250 nm) using Phosphorus ions at **190 keV** (interpolating between the two ranges shown). Close this window with the Table.
- Before leaving the *Stopping and Range* window, look at the other Help messages for the ***S & R Tables*** (press ? buttons).
- Press **Main Menu** button to return to the Home page of SRIM.

. *Damage Production by Phosphorus ions at 190 keV*

- On the Main Menu, there is a Help beside the button TRIM Calculation. Press this to read the Help, ? , for this program.
- TRIM (Transport of Ions in Matter) is a very complicated program that describes not only the range of ions into matter, but also details many other aspects of the damage done to the target during the slowing-down process. It will allow you to see the ions penetrating into the target with full animation, and also shows recoil cascades and target atoms mixing together. Is makes the calculation for one ion at a time, in order to make precise evaluations of the physics of each encounter between the ion and a target atom. This calculation may be time consuming – from a second to a few minutes for each ion. The accuracy is determined by the number of ions followed. Typically, a calculation for 1000 ions will give better than 10% accuracy.
- Click **Trim Calculation** on Main Menu

- The next window is for the TRIM Setup for the calculation. It contains more options than the simpler Table of Ranges, since we have to include many details about the target structure.
- Go to ION DATA and click on PT button. Select **Phosphorus**. Note that other ion parameters are automatically filled in.
- On this same ION DATA line, in the box under "Energy (keV)" enter **190**. This was the energy that we found using the SR Tables to put the Phosphorus peak about 250 nm deep into the silicon target.
- Go down to TARGET DATA. This window can get very complicated since we can have many target layers (up to 20) made up of complex compounds. We will study this in a later Tutorial, but we will only use a simple silicon substrate in this exercise.
- Find the PT button for the target. Open the Periodic Table window and select **Si**.
- Go to the LEFT side of this line, and for "*Width*" enter **3500 Ang**. This is the layer width of the target. Since we don't care what happens much deeper than 250 nm, this is an adequate target thickness.
- Go to the LEFT side of the TARGET DATA input, and for "*Layer Name*" enter "**Silicon**" (instead of *Layer 1*)
- Next we will consider what kind of calculation is needed. TRIM can be used for simple calculations such as used in the Stopping and Range (SR) Tables, which executes in less than a second, to detailed calculations of every interaction of the ions with the target, which may take a few hours to calculate 100 ions. The type of calculation is setup using the two drop-down menus under the title "Type of TRIM Calculation".
- Go to the TOP-RIGHT box "DAMAGE". On the right is the Help box, ? . Press this to read about the types of damage calculations that are available. Although it may seem complex, over the next lessons you will use most of these for special applications.
- Scroll down the DAMAGE to select "***Detailed Calculation with Full Damage Cascades***".
- Below this are Basic Plots which are available. You can ignore this for now. We will use various plots, but we will call them up during the calculation as needed.
- Finally, on the far right, near the middle of the window, near the boxes called "Damage (eV)" there is another Help box, ? . Look at this so you can see various energies that are needed to describe specific damage types. We will go into this in the next Tutorial, but you should begin to learn the terms: Displacement energy, Surface binding energy and Lattice binding energy.
- The setup is complete. Look at all the boxes to see if you can understand them. Press the Help buttons for explanations.
- Finally, press **Save Input and Run TRIM**

. *TRIM Calculation Results for Damage*

The TRIM calculation beings. There is a pause as TRIM generates internal tables which describe your target. Then you see the first ion track. The ion track shows a red dot wherever the ion creates a vacancy (knocks a silicon atom away from its lattice site). The green dots are vacancies caused by recoiling silicon atoms.

- Note that the ion creates damage constantly (red dots), while there are clusters of green dots where recoiling silicon atoms cause what is called a ***recoil cascade***.

- Every time the phosphorus hits a silicon atom hard, it will transfer a significant portion of its energy. This is true because the mass of P is almost the same as the mass of Si. If the ion / target atom masses are very different, then there is much less energy transferred to the target atom. This is basic physics of the elastic collision of two particles. Every time there is a hard ion/silicon hit, and a green cascade is formed, there is a good chance that the ion changes direction. Since you are only seeing two axes, some deflections may not be apparent.
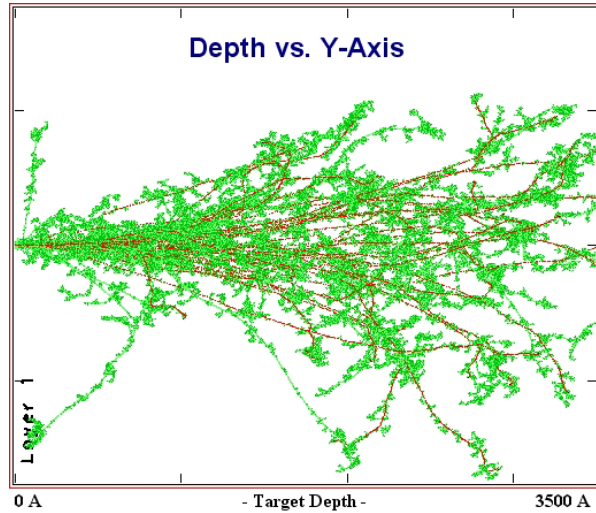
- Almost every time the ion has a collision with a target atom, there is one vacancy created (a red dot). The target atom then recoils and all its collisions which cause vacancies are plotted as green dots. A single recoil atom may cause up to a 1000 vacancies (green), while the ion only gets 1 vacancy plotted (red).
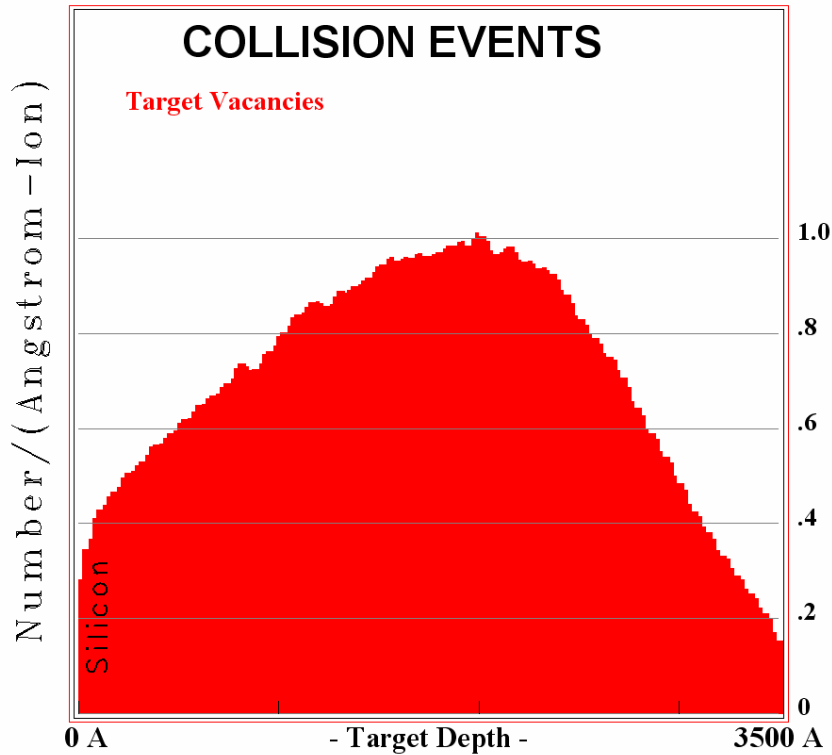
- On the left side of this *TRIM Calculation Window* are various buttons in a table called **DISTRIBUTIONS**. The left hand column of buttons, **?**, are *Help* for each of the plots. The second column of buttons, **File**, generate files on the hard disk (don't click them). The third column, **Plot**, (white squares) are for plots. We will use these for the bullet items below. When you click on any button, there is a pause until the calculation for the current ion completes. Then the command is executed. So you have to be patient. The calculation continues while you look at any plots, and these plots will be updated after each successive ion.
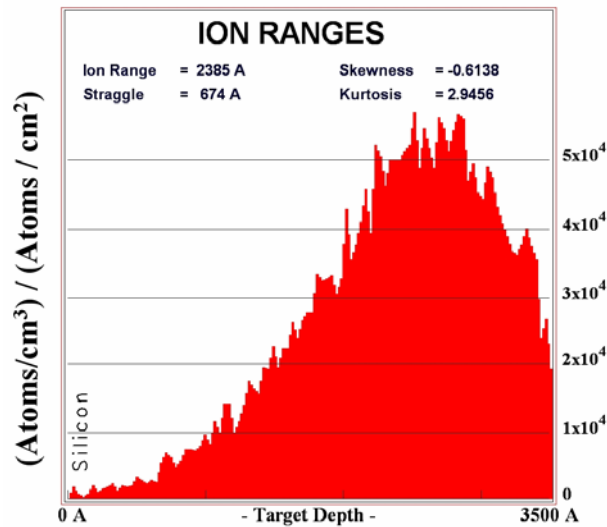
- The top plot is the **ION DISTRIBUTION**. Read the Help, **?**. The terms should be familiar to you. Now click on the plot box for this item. A plot will appear titled: **ION RANGES**. You will see the distribution of phosphorus ions (190 keV) building up in the silicon target. The "Ion Range" should be about 2400-2500 A. We set up the target depth at 3500A to be able to catch most of the ions in the plots. Note the Ordinate units: **"(Atoms/cm3)/ (Atoms/cm2)"**. Although these units appear strange, when you multiply by an implantation dose (ions/cm^2), you will end with the impurity concentration (atoms/cm^3) vs. depth. This is GOOD. You want a peak impurity concentration of ~5×10^{18}/cm^3. See if you can determine that an implant dose of 10^{14} phosphorus/cm^2 will be adequate. This is perfect doping for an n-well.
  - If you wanted a peak dopant concentration of 10^{17}/cm^3, what would be the required dose for the phosphorus implant? _____

- o Note that the higher moments of the distribution are also given on the plot (straggle, skewness, kurtosis). These are briefly discussed in the Help for the plot. For more details, click on the top tab "Help, FAQ and Scientific Explanations", then "TRIM FAQ and Solutions", then "Statistics of Range Distributions". Read this to get an understanding that these range terms are various statistical methods which describe the final ion distribution.
  - o Close this Range plot window (every open plot window slows down the calculation).

- Next we will look at the **Ion/Recoil Distribution**. Press the Help ? button for a description. At the bottom of this Help window is a copy of a typical harddisk file. [1]

- Select the plot for the **Ion/Recoil Distribution.** Note that the "Ion" plot (red) is identical to that shown in the Ion Distribution. The green plot shows the silicon recoil distribution. These are all the silicon atoms knocked out of their lattice sites, creating vacancies. Note that the distribution of silicon recoils (green) has a shallower peak than that for the phosphorus ions. Near the end of the phosphorus tracks, the ions do not have enough energy to create massive cascades. The two peaks are about the same size, so they both contribute about equally to the total damage to the target.

- The units of this plot are also **"(Atoms/cm3)/ (Atoms/cm2)"**. Near the peak of the Si recoil distribution, the value is 10^8. The density of silicon is about 5×10^{22} atoms/cm^3. With a little math, you can derive that for a dose of 5×10^{14} P atoms/cm^2, you will average one displacement per target atom at the peak of the damage distribution. This would indicate that a crystal target should go amorphous, except at room-temperature about 99% of the silicon crystal damage almost instantly anneals and most of this damage disappears. This will be discussed in more detail below.

- A second plot will help you to understand details of these collisions. The plot called "Collision Events" plots the number of Target Vacancies as a function of depth (the plot is generated by clicking on *Damage Events* in the TRIM Calculation window and selecting *Total Vacancies*). Note that the peak also is about 1.0 vacancies per Å-ion, in agreement with the Recoil distribution on the previous figure (10^8Å = 1 cm). This subject will be covered in more detail in Tutorial #4.

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[1] Note: If the characters in this datafile look weird, then the font "*MS-LineDraw*" has not been installed on your PC. This must be done before you continue. It has been included in the SRIM software, and has been put into the directory: *C:/WINDOWS/FONTS*. Use Windows Explorer to find it. Select it, and press *FILE* and then "*INSTALL NEW FONT*". These instructions may vary with different editions of *Windows*.

COLLISION EVENTS

Target Vacancies

Number/(Angstrom–Ion)

Silicon

1.0
.8
.6
.4
.2
0

0 A   - Target Depth -   3500 A

. *Does the Phosphorus Create an Amorphous Layer ?*

We can estimate whether the phosphorus can create an amorphous layer. At the PEAK of the damage plot created above, the vacancy rate is about 1 vacancy/target atom. But we are assuming that 99% of the damage instantly anneals, leaving only 1% damage. Using the above plot, with an implant dose of 10^{15}/cm^2 ions, that makes 10^{13} stable vacancies / Angstrom-cm^2. Converting this, using: 10^8 Angstrom $\equiv$ 1 cm, gives a vacancy density of 10^{21} vacancies/cm^3.

The density of silicon is 5×10^{22} atoms/cm^3. The calculated damage is 10^{21} vacancies/cm^3. Hence the silicon target is damaged to about 2%, and the implant layer is not amorphous. This conclusion is not quite accurate because the displacement energy for silicon (discussed in Tutorial-4) will decrease as damage accumulates. This means that once you have partial damage, it is easier to create more damage because the lattice is more loosely coupled and atoms are easier to dislodge. These changes in the crystal integrity are not included in TRIM, so the damage may be underestimated.