Introduction of SRIM Tutorials

Simulation Section of Nuclear Materials Experiment

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2017-04-05
2017-04-10

Outline

Tutorial 1:
Introduction to Ion Ranges, Does and Damage

Tutorial 2:
Target Mixing and Sputtering

Tutorial 3:
Building Complex Targets

Tutorial 4:
Calculations of Target Damage

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Tutorial 1:
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SRIM Tutorials 1: Introduction to Ion Ranges, Does and Damage

➢ Objective

To find the energy and dose of ions required to implant atoms into a target at given depth and concentration.

➢ Case

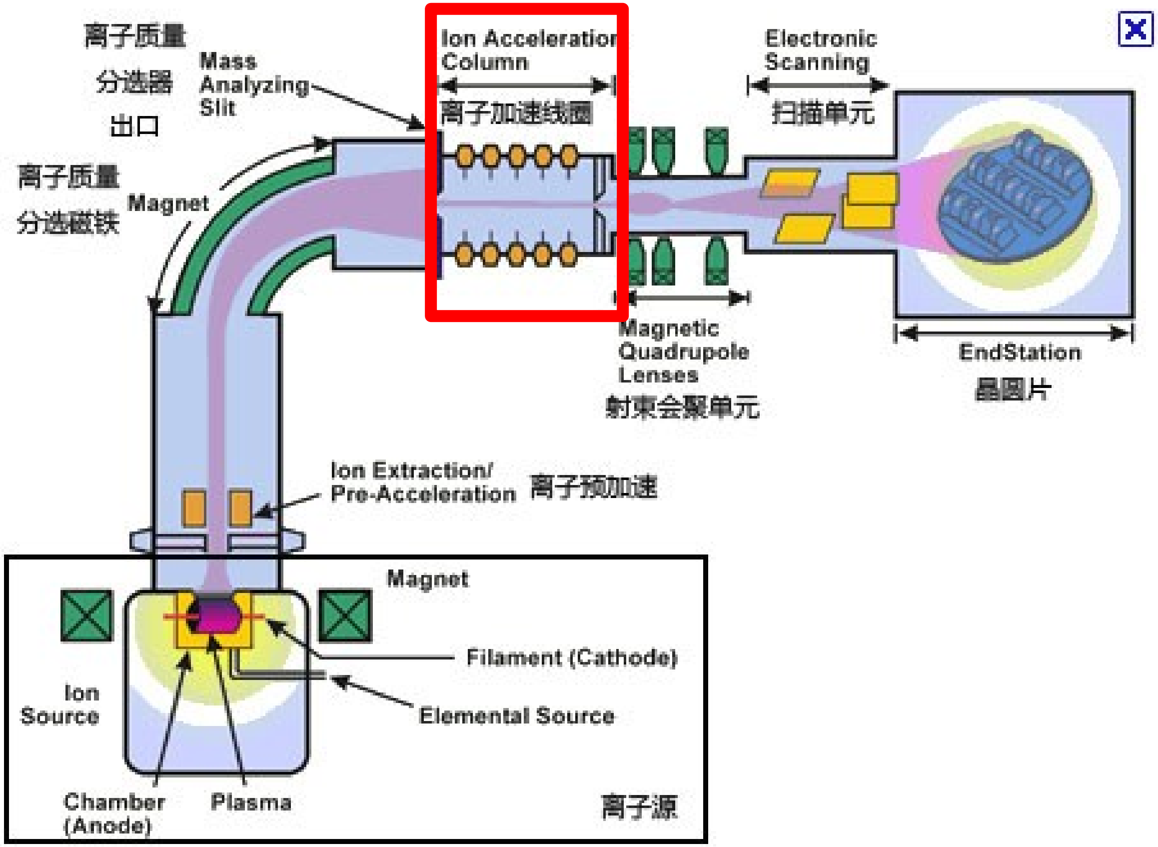
To simulate the implantation of n-well of a CMOS semiconductor device.

➢ Parameters

1. **Ions: N-type dopant-Phosphorus(P)/ Arsenic(As)/ Antimony(Sb) (VB);**
2. **Target: Silicon;**
3. **Peak concentration depth: 250 nm;**
4. **Peak dopant concentration: 5×10^{18} atoms/cm^3.**

➢ Experimental condition

The maximum energy of the accelerator is limited to 200 keV.

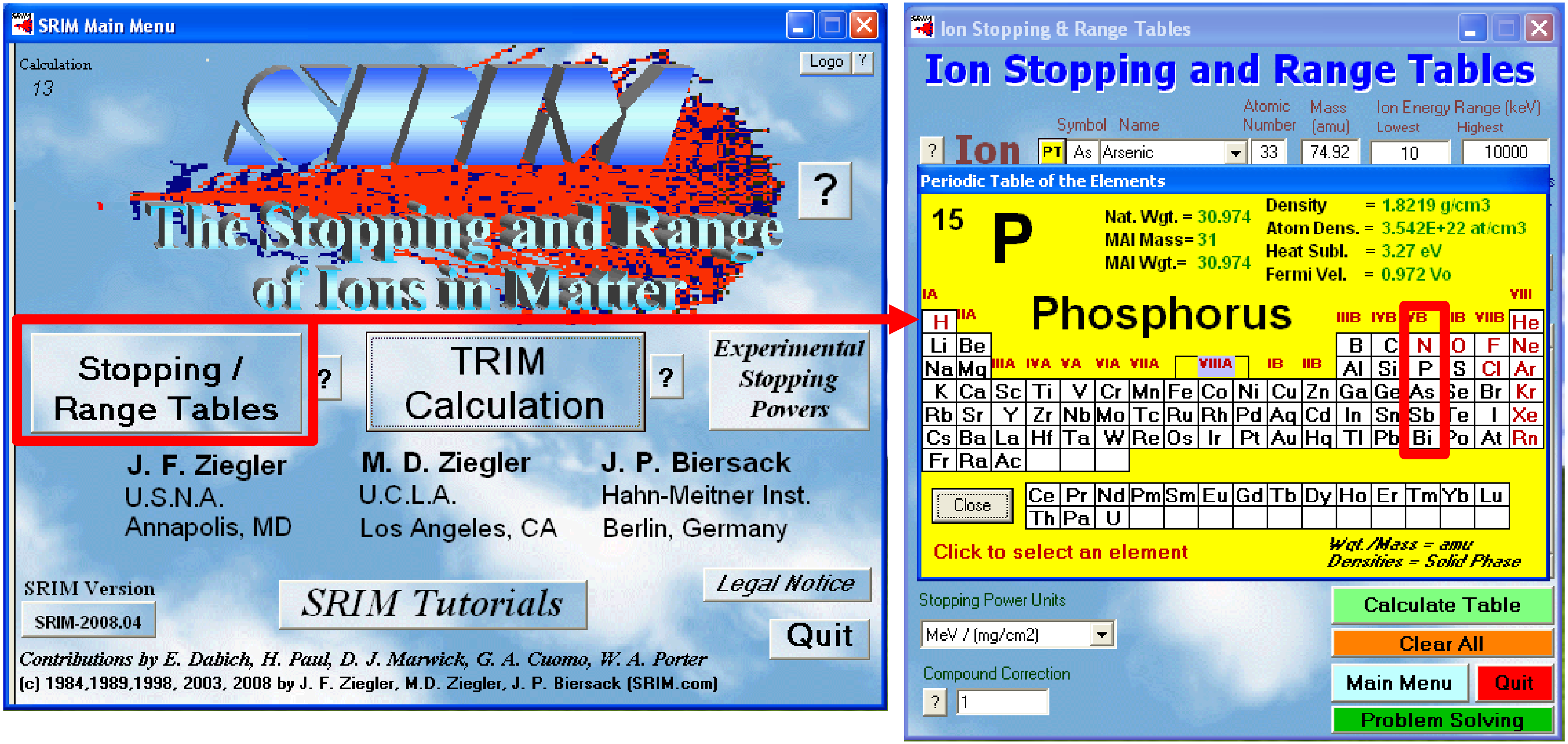


➢ Questions

1. **Which element will your use and how to set its energy?**
2. **What dose is required (ions/cm^2)?**
3. **Will the target be amorphous after the implant?**

➢ Element and energy of implanted ion

Recall the implanted ion should be chosen from VB column in periodic table and the peak concentration depth is 250 nm.



Calculation 13

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SRIM Version: SRIM-2008.04

Contributions by E. Dabich, H. Paul, D. J. Marwick, G. A. Cuomo, W. A. Porter

(c) 1984,1989,1998, 2003, 2008 by J. F. Ziegler, M.D. Ziegler, J. P. Biersack (SRIM.com)

	Symbol	Name	Atomic Number	Mass (amu)	Ion Energy Range (keV) Lowest	Highest
Ion	As	Arsenic	33	74.92	10	10000

15 P Phosphorus

Nat. Wgt. = 30.974
MAI Mass= 31
MAI Wgt.= 30.974
Density = 1.8219 g/cm3
Atom Dens. = 3.542E+22 at/cm3
Heat Subl. = 3.27 eV
Fermi Vel. = 0.972 Vo

Wgt./Mass = amu
Densities = Solid Phase

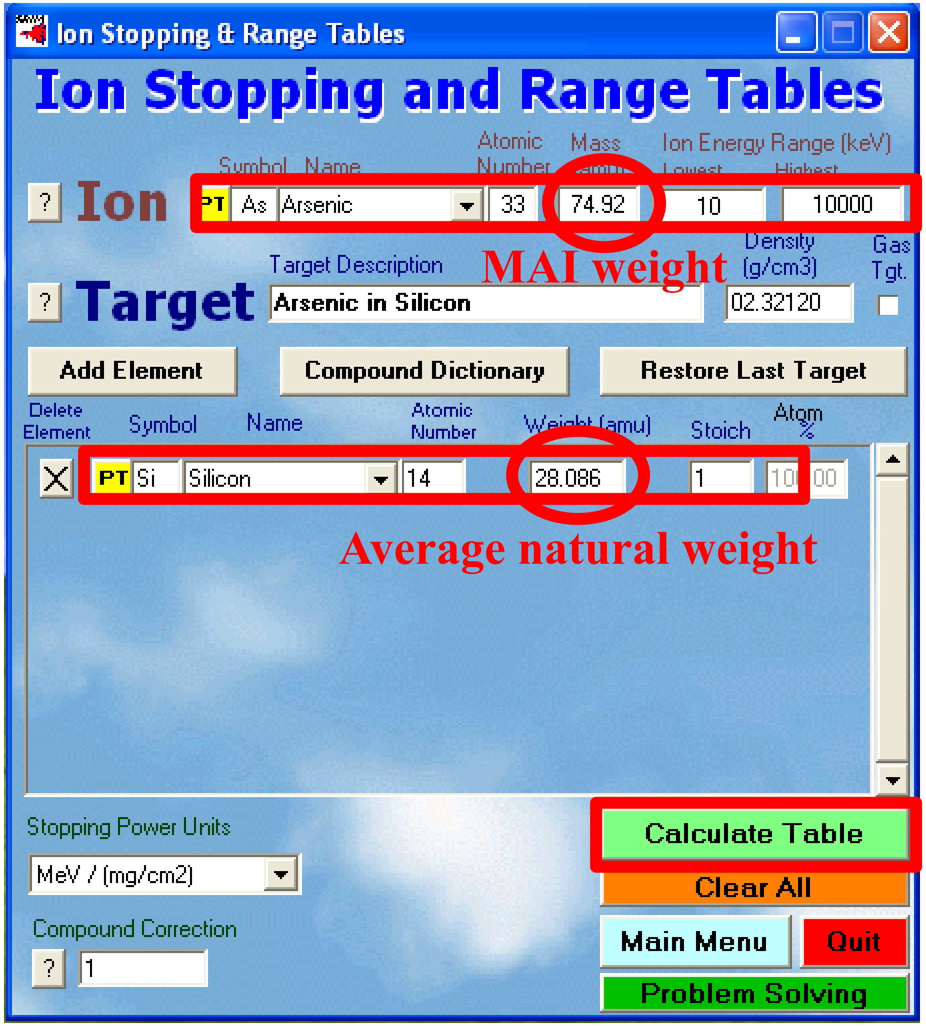
Stopping Power Units: MeV / (mg/cm2)

Compound Correction: 1

First, the As is chosen as implanted ion.

SRIM Tutorials 1

The target is silicon.



Ion Stopping and Range Tables

Ion: Symbol As, Name Arsenic, Atomic Number 33, Mass (amu) 74.92, Ion Energy Range (keV) Lowest 10, Highest 10000

MAI weight

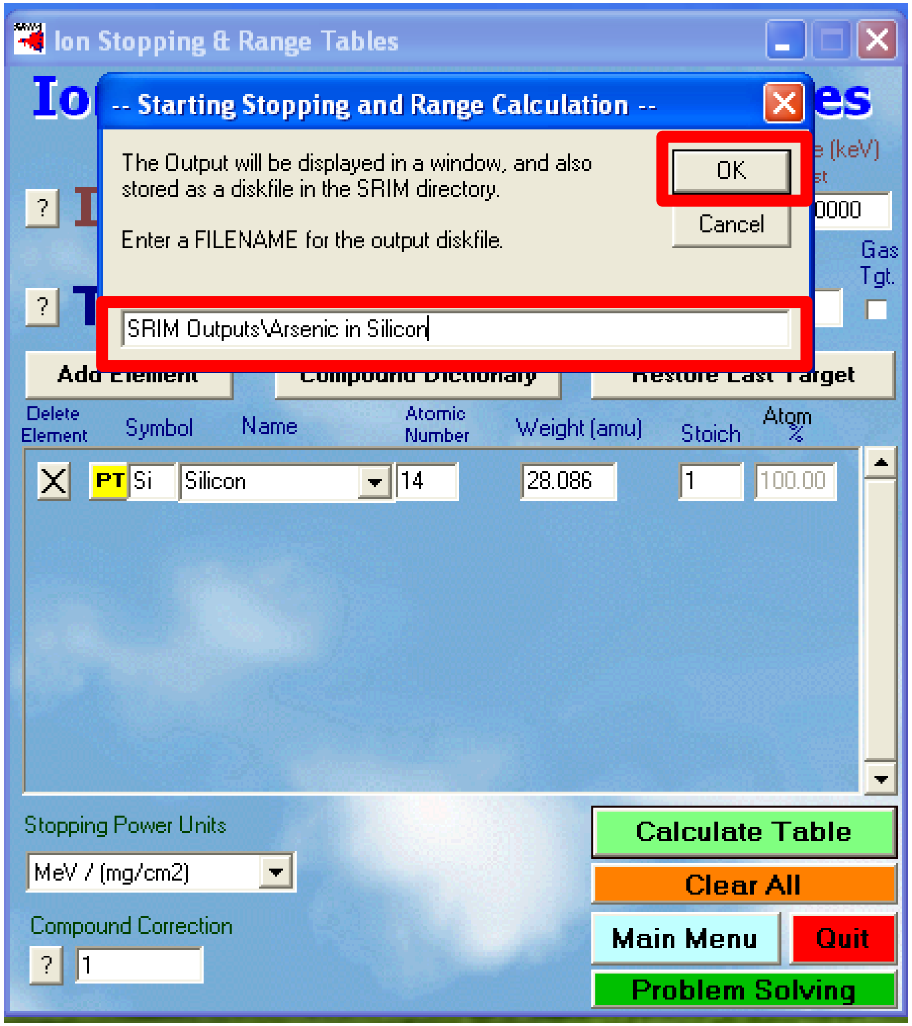
Target: Target Description Arsenic in Silicon, Density (g/cm3) 02.32120, Gas Tgt. ☐

Symbol	Name	Atomic Number	Weight (amu)	Stoich	Atom %
Si	Silicon	14	28.086	1	100.00

Average natural weight

Stopping Power Units: MeV / (mg/cm2)

Compound Correction: 1



-- Starting Stopping and Range Calculation --

The Output will be displayed in a window, and also stored as a diskfile in the SRIM directory.

Enter a FILENAME for the output diskfile.

SRIM Outputs\Arsenic in Silicon

The default name of the output file is set by element name of ion and target.

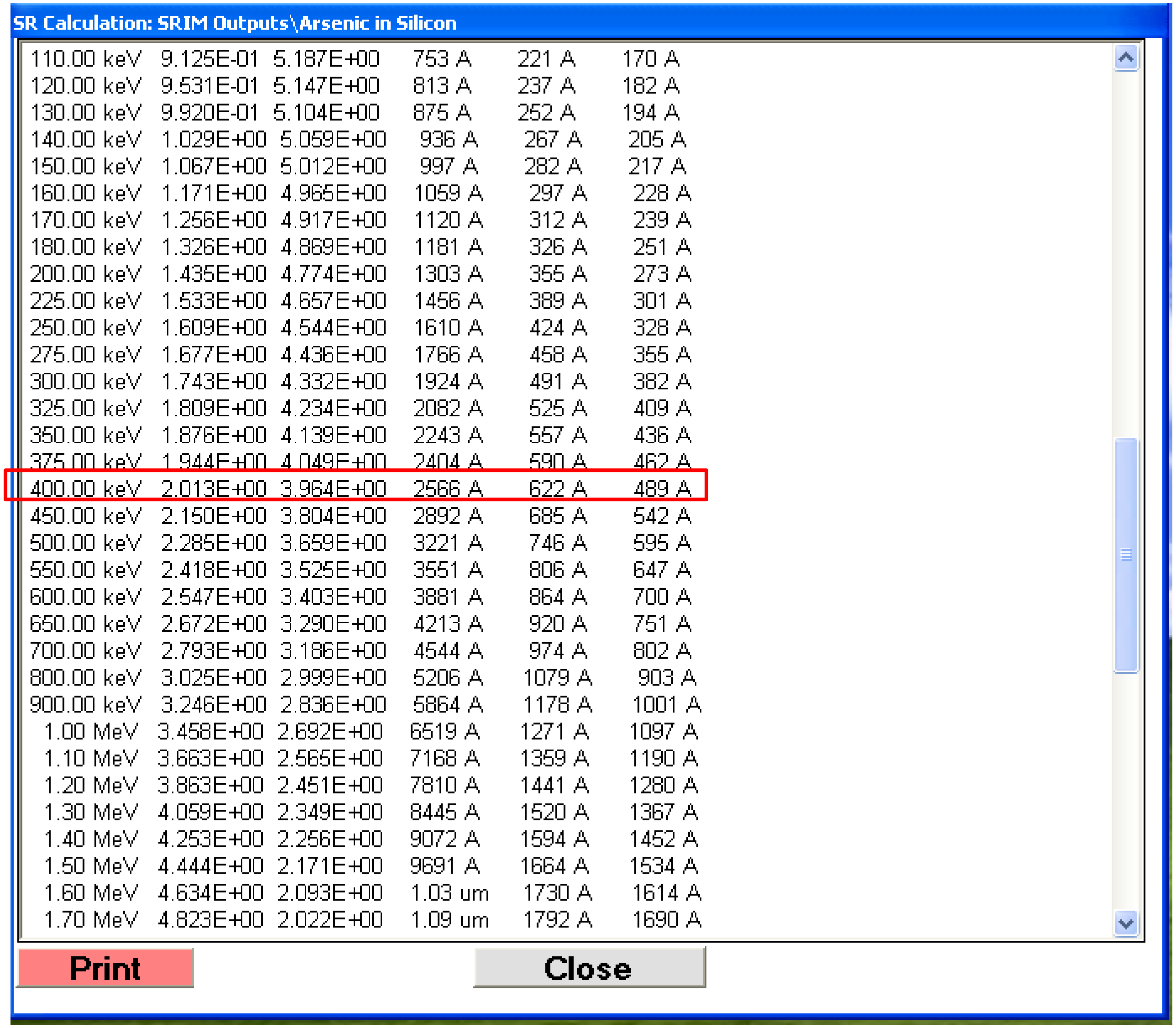
SRIM Tutorials 1

To reach the peak concentration depth 250 nm, the energy of implanted ion As should be up to 400 keV.

Conclusion:

This is a higher energy than your 200 keV implanter can reach.

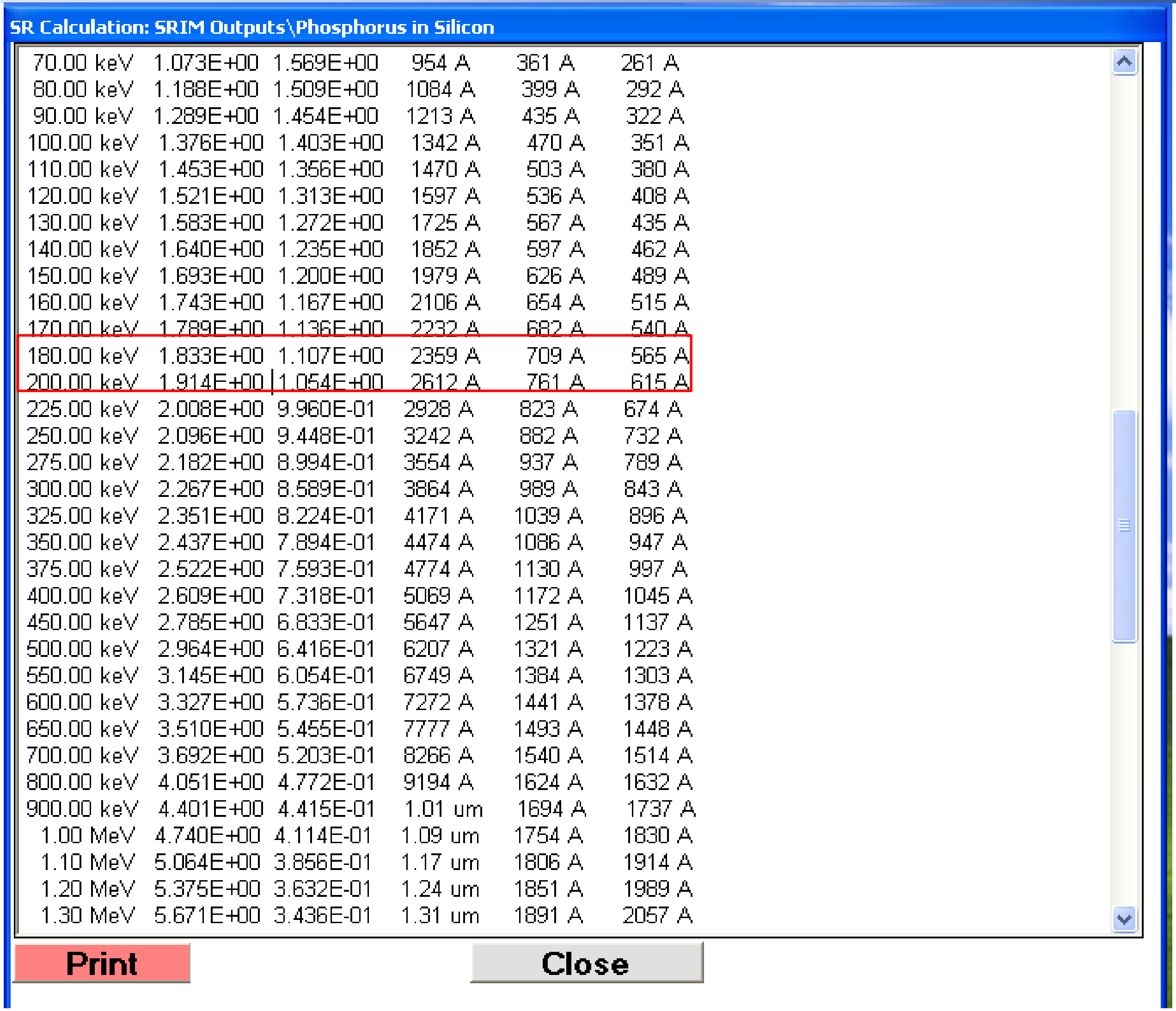
Then Recalculate the Range Tables using P as implanted ions.



SR Calculation: SRIM Outputs\Arsenic in Silicon

```
110.00 keV  9.125E-01  5.187E+00   753 A    221 A    170 A
120.00 keV  9.531E-01  5.147E+00   813 A    237 A    182 A
130.00 keV  9.920E-01  5.104E+00   875 A    252 A    194 A
140.00 keV  1.029E+00  5.059E+00   936 A    267 A    205 A
150.00 keV  1.067E+00  5.012E+00   997 A    282 A    217 A
160.00 keV  1.171E+00  4.965E+00  1059 A    297 A    228 A
170.00 keV  1.256E+00  4.917E+00  1120 A    312 A    239 A
180.00 keV  1.326E+00  4.869E+00  1181 A    326 A    251 A
200.00 keV  1.435E+00  4.774E+00  1303 A    355 A    273 A
225.00 keV  1.533E+00  4.657E+00  1456 A    389 A    301 A
250.00 keV  1.609E+00  4.544E+00  1610 A    424 A    328 A
275.00 keV  1.677E+00  4.436E+00  1766 A    458 A    355 A
300.00 keV  1.743E+00  4.332E+00  1924 A    491 A    382 A
325.00 keV  1.809E+00  4.234E+00  2082 A    525 A    409 A
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
550.00 keV  2.418E+00  3.525E+00  3551 A    806 A    647 A
600.00 keV  2.547E+00  3.403E+00  3881 A    864 A    700 A
650.00 keV  2.672E+00  3.290E+00  4213 A    920 A    751 A
700.00 keV  2.793E+00  3.186E+00  4544 A    974 A    802 A
800.00 keV  3.025E+00  2.999E+00  5206 A   1079 A    903 A
900.00 keV  3.246E+00  2.836E+00  5864 A   1178 A   1001 A
  1.00 MeV  3.458E+00  2.692E+00  6519 A   1271 A   1097 A
  1.10 MeV  3.663E+00  2.565E+00  7168 A   1359 A   1190 A
  1.20 MeV  3.863E+00  2.451E+00  7810 A   1441 A   1280 A
  1.30 MeV  4.059E+00  2.349E+00  8445 A   1520 A   1367 A
  1.40 MeV  4.253E+00  2.256E+00  9072 A   1594 A   1452 A
  1.50 MeV  4.444E+00  2.171E+00  9691 A   1664 A   1534 A
  1.60 MeV  4.634E+00  2.093E+00  1.03 um  1730 A   1614 A
  1.70 MeV  4.823E+00  2.022E+00  1.09 um  1792 A   1690 A
```

Phosphorus in Silicon



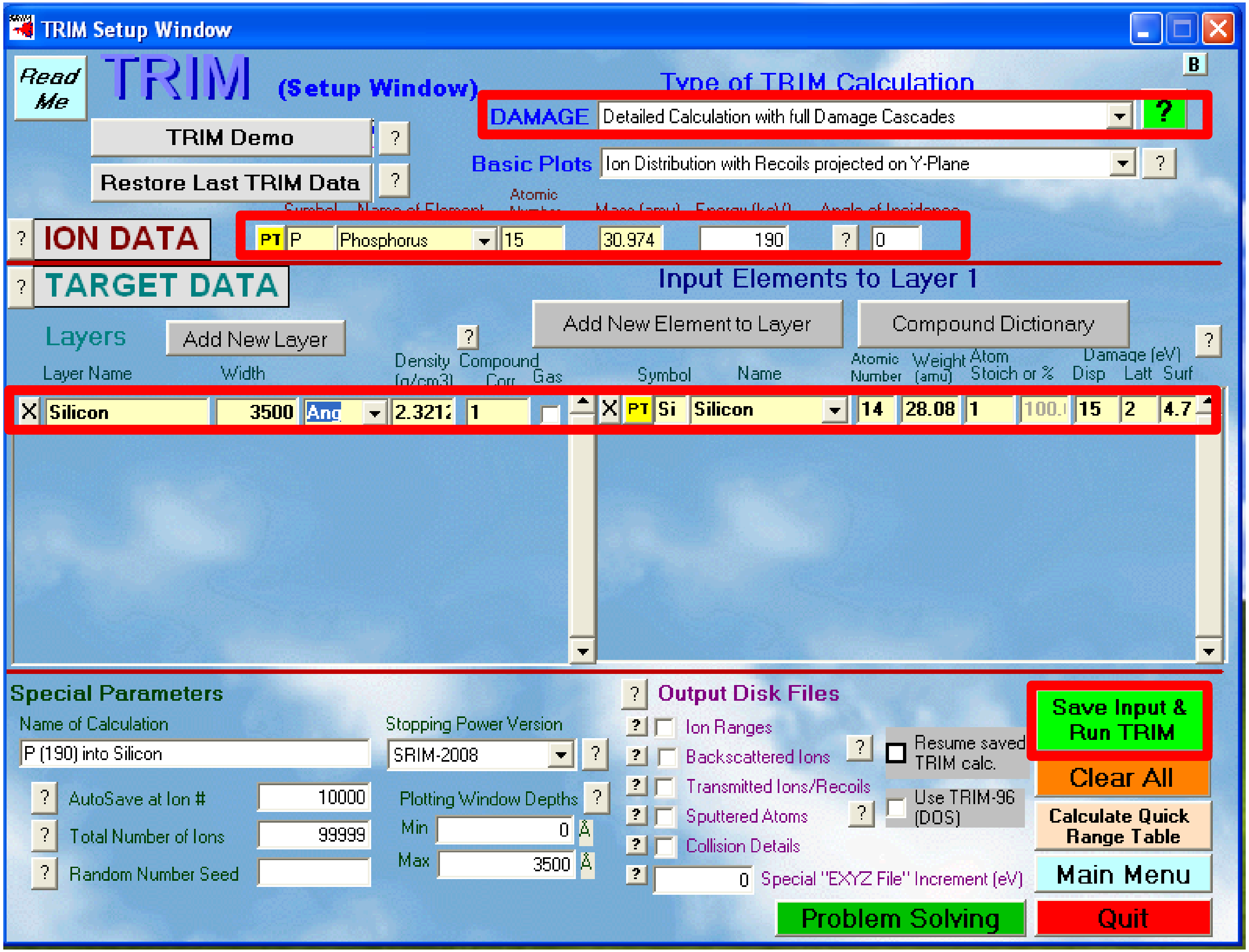
SR Calculation: SRIM Outputs\Phosphorus in Silicon

```
 70.00 keV  1.073E+00  1.569E+00    954 A      361 A      261 A
 80.00 keV  1.188E+00  1.509E+00   1084 A      399 A      292 A
 90.00 keV  1.289E+00  1.454E+00   1213 A      435 A      322 A
100.00 keV  1.376E+00  1.403E+00   1342 A      470 A      351 A
110.00 keV  1.453E+00  1.356E+00   1470 A      503 A      380 A
120.00 keV  1.521E+00  1.313E+00   1597 A      536 A      408 A
130.00 keV  1.583E+00  1.272E+00   1725 A      567 A      435 A
140.00 keV  1.640E+00  1.235E+00   1852 A      597 A      462 A
150.00 keV  1.693E+00  1.200E+00   1979 A      626 A      489 A
160.00 keV  1.743E+00  1.167E+00   2106 A      654 A      515 A
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
250.00 keV  2.096E+00  9.448E-01   3242 A      882 A      732 A
275.00 keV  2.182E+00  8.994E-01   3554 A      937 A      789 A
300.00 keV  2.267E+00  8.589E-01   3864 A      989 A      843 A
325.00 keV  2.351E+00  8.224E-01   4171 A     1039 A      896 A
350.00 keV  2.437E+00  7.894E-01   4474 A     1086 A      947 A
375.00 keV  2.522E+00  7.593E-01   4774 A     1130 A      997 A
400.00 keV  2.609E+00  7.318E-01   5069 A     1172 A     1045 A
450.00 keV  2.785E+00  6.833E-01   5647 A     1251 A     1137 A
500.00 keV  2.964E+00  6.416E-01   6207 A     1321 A     1223 A
550.00 keV  3.145E+00  6.054E-01   6749 A     1384 A     1303 A
600.00 keV  3.327E+00  5.736E-01   7272 A     1441 A     1378 A
650.00 keV  3.510E+00  5.455E-01   7777 A     1493 A     1448 A
700.00 keV  3.692E+00  5.203E-01   8266 A     1540 A     1514 A
800.00 keV  4.051E+00  4.772E-01   9194 A     1624 A     1632 A
900.00 keV  4.401E+00  4.415E-01   1.01 um    1694 A     1737 A
  1.00 MeV  4.740E+00  4.114E-01   1.09 um    1754 A     1830 A
  1.10 MeV  5.064E+00  3.856E-01   1.17 um    1806 A     1914 A
  1.20 MeV  5.375E+00  3.632E-01   1.24 um    1851 A     1989 A
  1.30 MeV  5.671E+00  3.436E-01   1.31 um    1891 A     2057 A
```

This table shows that we can implant the n-well with a peak at 2500 Å (250 nm) using Phosphorus ions at 190 keV (interpolating between the two ranges shown).

SRIM Tutorials 1

➢ TRIM setup



DAMAGE: Detailed Calculation with full Damage Cascades

Basic Plots: Ion Distribution with Recoils projected on Y-Plane

ION DATA

Symbol	Name of Element	Atomic Number	Mass (amu)	Energy (keV)	Angle of Incidence
P	Phosphorus	15	30.974	190	0

TARGET DATA

Layer Name	Width		Density (g/cm3)	Compound Corr	Gas
Silicon	3500	Ang	2.321	1	☐

Input Elements to Layer 1

Symbol	Name	Atomic Number	Weight (amu)	Atom Stoich	or %	Damage (eV) Disp	Latt	Surf
Si	Silicon	14	28.08	1	100.	15	2	4.7

Special Parameters

Name of Calculation: P (190) into Silicon

Stopping Power Version: SRIM-2008

AutoSave at Ion # 10000

Total Number of Ions 99999

Random Number Seed

Plotting Window Depths
Min 0 Å
Max 3500 Å

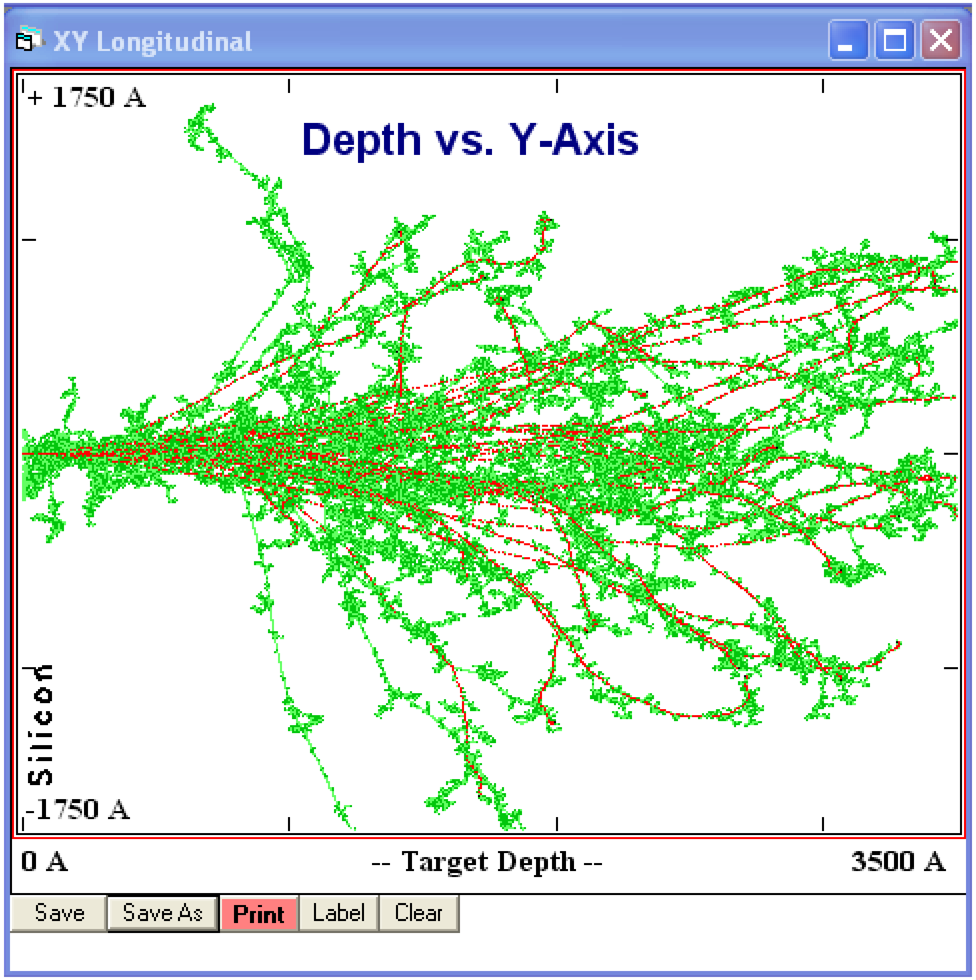
Output Disk Files

- ☐ Ion Ranges
- ☐ Backscattered Ions
- ☐ Transmitted Ions/Recoils
- ☐ Sputtered Atoms
- ☐ Collision Details
- 0 Special "EXYZ File" Increment (eV)

☐ Resume saved TRIM calc.

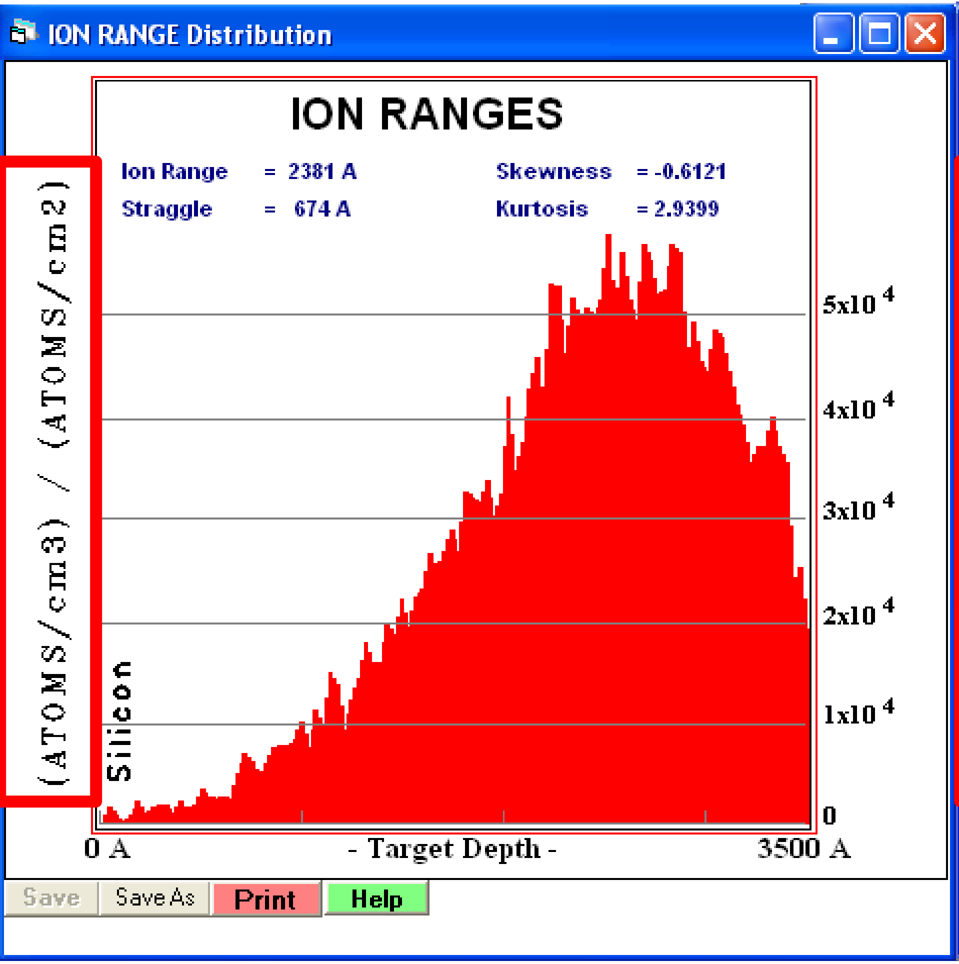
☐ Use TRIM-96 (DOS)

Trajectories of ions and recoil atoms



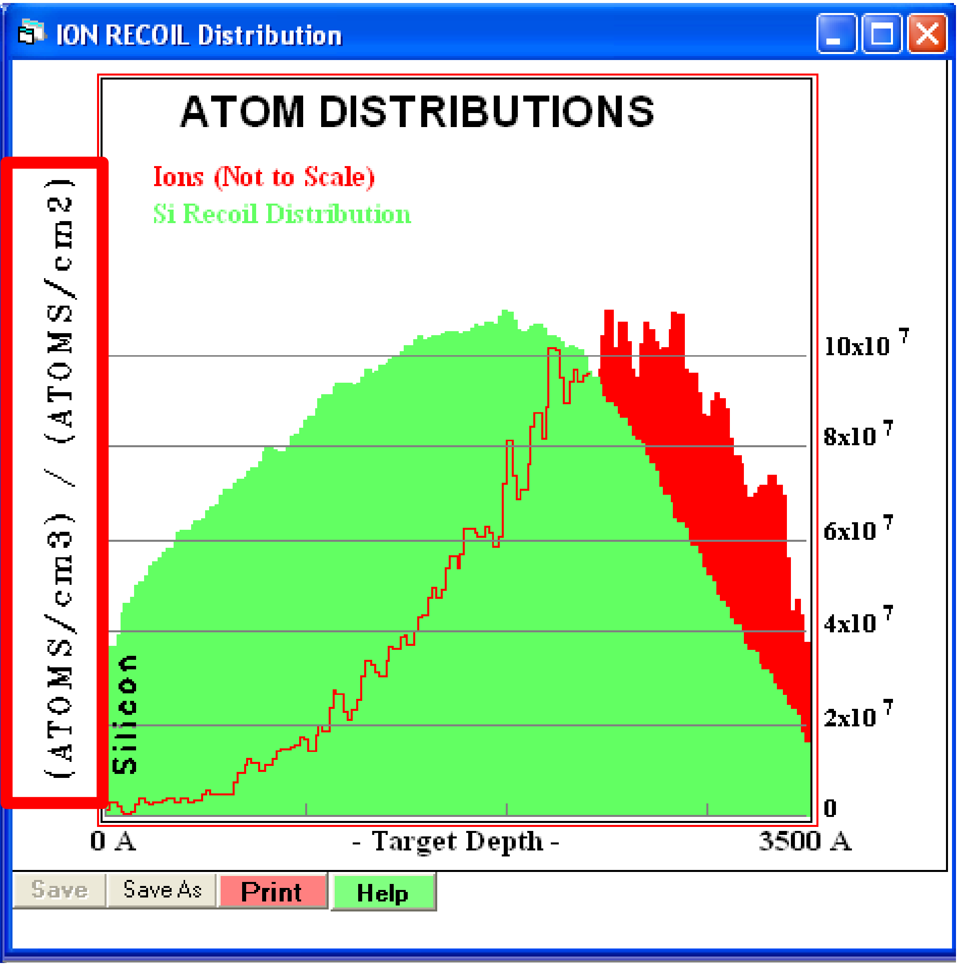
The ion track shows a red dot wherever the ion creates a vacancy (knocks a silicon atom away from its lattice site). The green dots are vacancies caused by recoiling silicon atoms.

Distribution of ions and recoil atoms


ION RANGE Distribution

ION RANGES

Ion Range = 2381 A
Straggle = 674 A
Skewness = -0.6121
Kurtosis = 2.9399


ION RECOIL Distribution

ATOM DISTRIBUTIONS

Ions (Not to Scale)
Si Recoil Distribution

$$\frac{Atoms/cm^3}{Atoms/cm^2} * \left(ions/cm^2\right) = Atoms/cm^3$$

SRIM Tutorials 1

Implanted dose of P

Recall we need the peak dopant concentration is 5x10^{18} atoms/cm^3.

According to the distribution of ions:
The peak concentration is 5x10^4 (atoms/cm^3)/ (atoms/cm^2).

So the final implanted dose we required is
5x10^{18}/ 5x10^4= 10^{14} ions/cm^2.

Will the target be amorphous after the implant?

We noticed that the peak concentration of recoil atoms is 10^8 (atoms/cm^3)/ (atoms/cm^2).

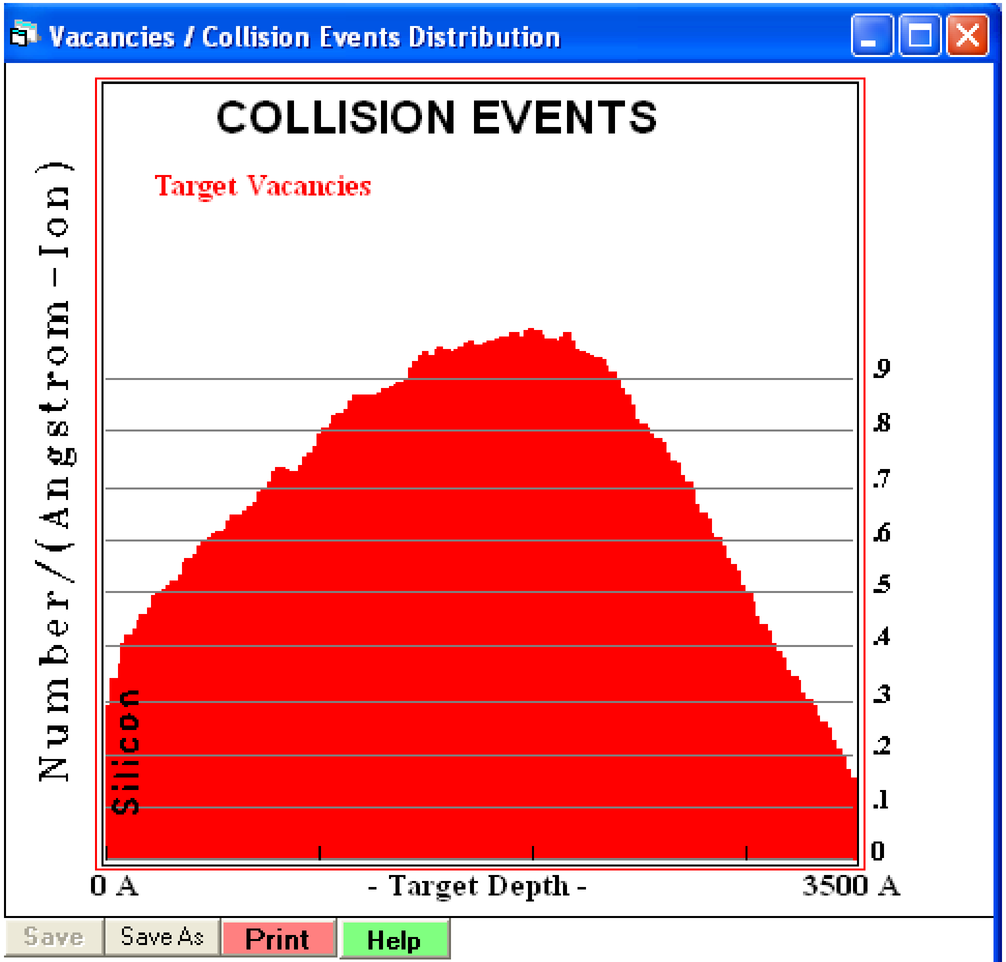
When the implanted dose of P is 5x10^{14} ions/cm^2, the concentration of displaced silicon atoms near peak is 5x10^{22} atoms/cm^3.

Recall the density of silicon is about 5x10^{22} atoms/cm^3.

It indicated that under this dose, all atom at peak of damage distribution will be displaced once.

SRIM Tutorials 1

Damage Events



The number of vacancies at peak is about 1.0 vacancies/Å-Ion.

1.0 vacancies/Å-Ion =
10^8 vacancies/cm-Ion

Assuming that 99% of the damage instantly anneals (i.e. leaving only 1% damage) and the implant dose is 10^{15} ions/cm^2, the total vacancies is
10^8 vacancies/cm-Ion* 10^{15} ions/cm^2 =
10^{23} vacancies/cm^3

Based on that only 1% was retained,
The final stable vacancies density is
10^{21} vacancies/cm^3

The damage degree of silicon is about 2%.

- Total displacements

移位碰撞的数目表明有多少靶原子在级联过程中离开原来的晶格位置。

- Total vacancies

靶中空位的数目表明靶原子离开原来的晶格位置而留下空位的数目。

- Replacement collisions

复位碰撞 运动的原子将晶格原子撞出后因能量降低，留在晶格位置，不产生空位 。

Displacements = Vacancies + Replacement Collisions

移位原子=空位+复合碰撞

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

空位=间隙原子+离开靶的原子

Outline

Tutorial 1:
Introduction to Ion Ranges, Does and Damage

Tutorial 2:
Target Mixing and Sputtering

Tutorial 3:
Building Complex Targets

Tutorial 4:
Calculations of Target Damage

SRIM Tutorials 2： Target Mixing and Sputtering

Physical background

- Interface Mixing

The transport of atoms from one layer of a target into another layer.

- Recoil implantation

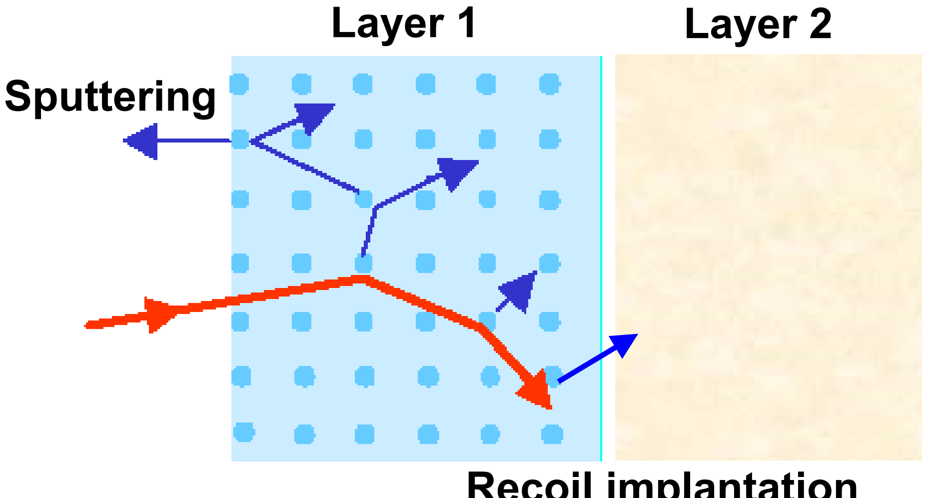
The process of recoil mixing is used to modify materials on purpose.

- Sputtering

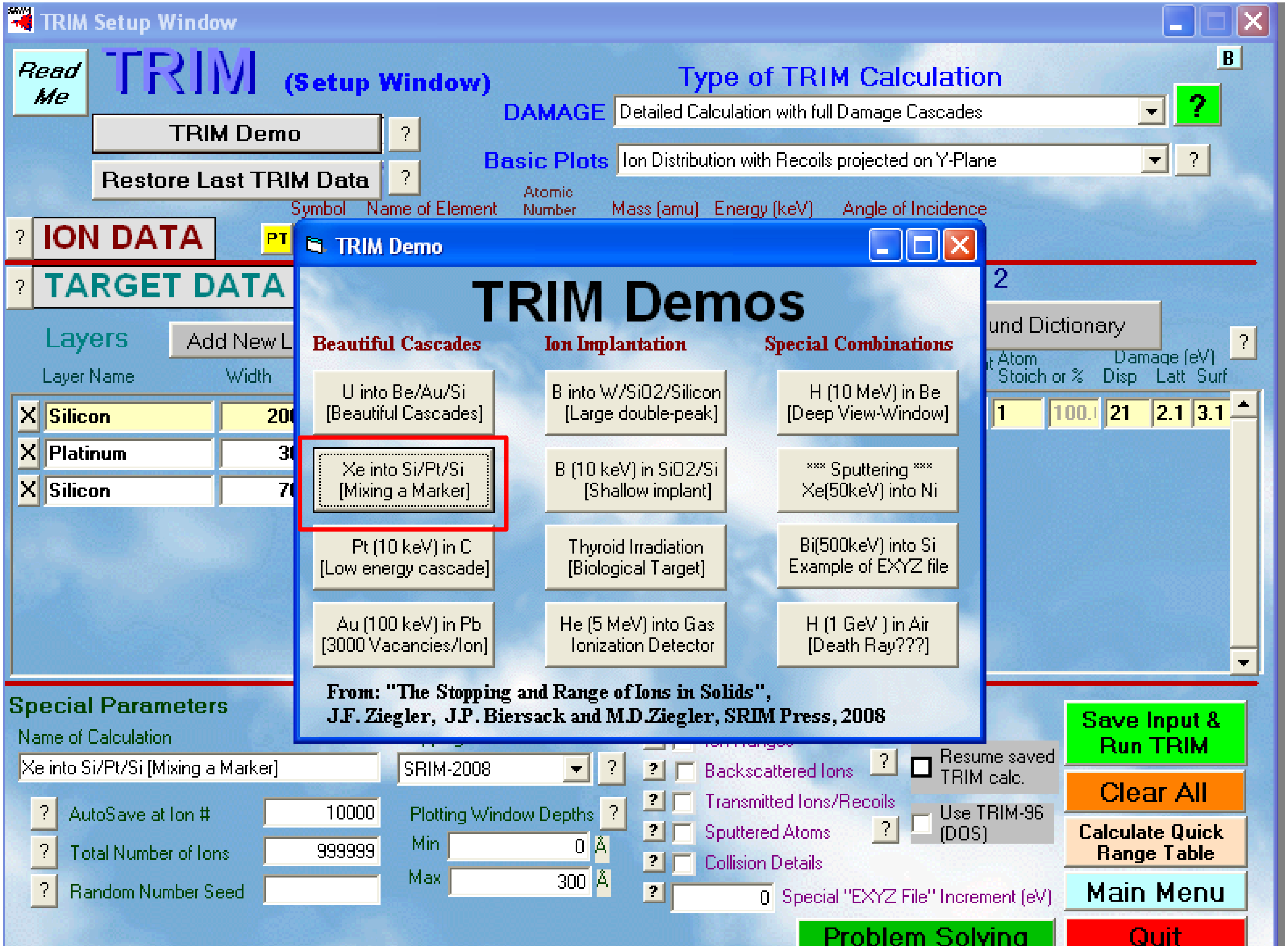
The opposite of Recoil Implantation. Here, surface atoms are removed from the target by creating recoil cascades that come back out of the target, and which give surface atoms enough energy so that they are driven away from the target.

- Sputtering yield

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



➤ TRIM Demo



Type of TRIM Calculation

DAMAGE: Detailed Calculation with full Damage Cascades

Basic Plots: Ion Distribution with Recoils projected on Y-Plane

Symbol | Name of Element | Atomic Number | Mass (amu) | Energy (keV) | Angle of Incidence

Layer Name	Width
Silicon	20
Platinum	3
Silicon	7

Atom Stoich or % | Damage (eV) Disp | Latt | Surf
1 | 100. | 21 | 2.1 | 3.1

TRIM Demo

TRIM Demos

Beautiful Cascades	Ion Implantation	Special Combinations
U into Be/Au/Si [Beautiful Cascades]	B into W/SiO2/Silicon [Large double-peak]	H (10 MeV) in Be [Deep View-Window]
Xe into Si/Pt/Si [Mixing a Marker]	B (10 keV) in SiO2/Si [Shallow implant]	*** Sputtering *** Xe(50keV) into Ni
Pt (10 keV) in C [Low energy cascade]	Thyroid Irradiation [Biological Target]	Bi(500keV) into Si Example of EXYZ file
Au (100 keV) in Pb [3000 Vacancies/Ion]	He (5 MeV) into Gas Ionization Detector	H (1 GeV) in Air [Death Ray???]

From: "The Stopping and Range of Ions in Solids", J.F. Ziegler, J.P. Biersack and M.D.Ziegler, SRIM Press, 2008

Special Parameters

Name of Calculation: Xe into Si/Pt/Si [Mixing a Marker]

SRIM-2008

AutoSave at Ion #: 10000

Total Number of Ions: 999999

Random Number Seed:

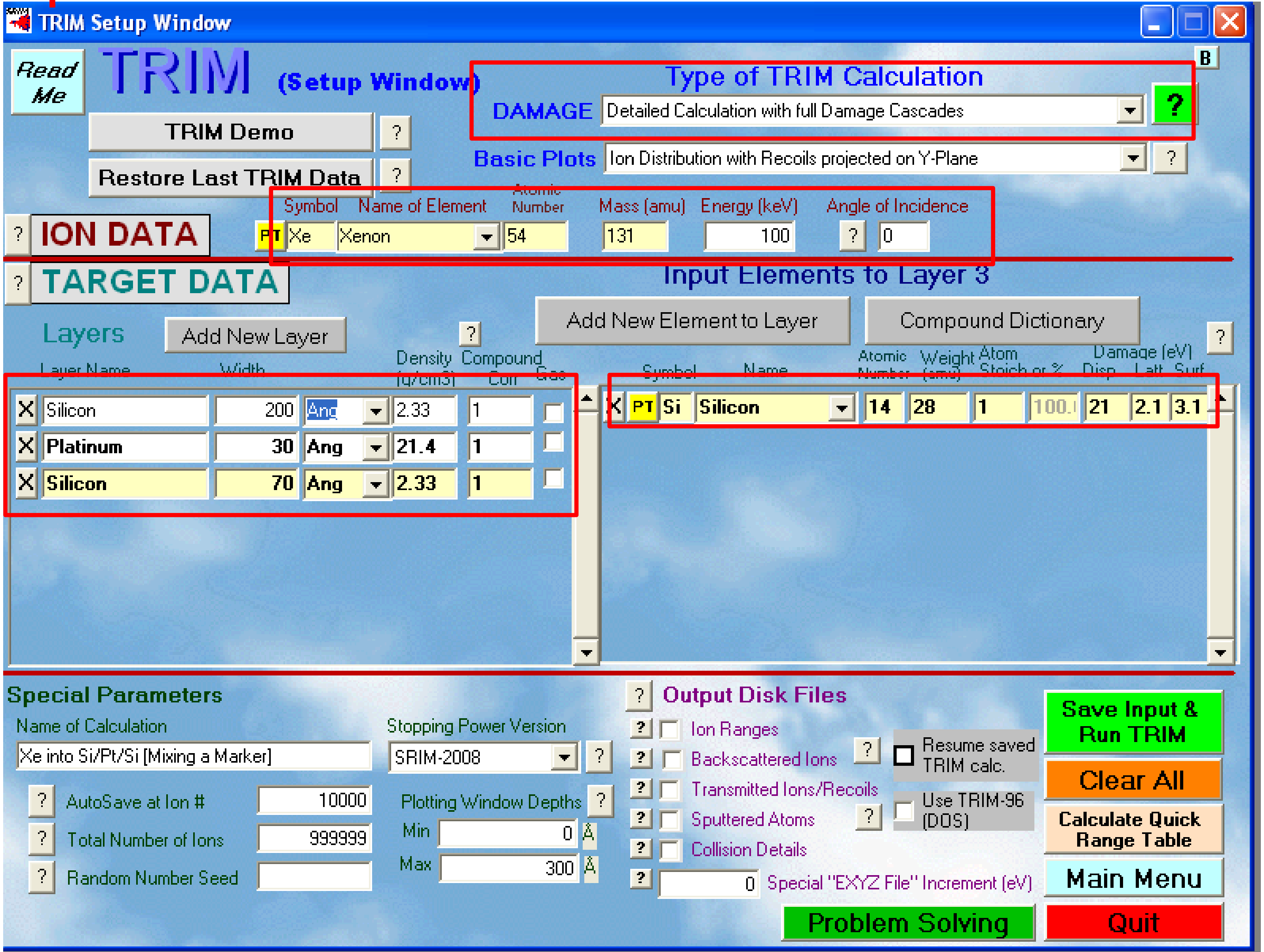
Plotting Window Depths: Min 0 Å, Max 300 Å

☐ Backscattered Ions
☐ Transmitted Ions/Recoils
☐ Sputtered Atoms
☐ Collision Details
0 Special "EXYZ File" Increment (eV)

☐ Resume saved TRIM calc.
☐ Use TRIM-96 (DOS)

SRIM Tutorials 2

➢ TRIM setup



Type of TRIM Calculation

DAMAGE: Detailed Calculation with full Damage Cascades

Basic Plots: Ion Distribution with Recoils projected on Y-Plane

ION DATA

Symbol	Name of Element	Atomic Number	Mass (amu)	Energy (keV)	Angle of Incidence
Xe	Xenon	54	131	100	0

TARGET DATA

Input Elements to Layer 3

Layers

	Layer Name	Width		Density (g/cm3)	Compound Corr	Gas
X	Silicon	200	Ang	2.33	1	☐
X	Platinum	30	Ang	21.4	1	☐
X	Silicon	70	Ang	2.33	1	☐

		Symbol	Name	Atomic Number	Weight (amu)	Atom Stoich	or %	Damage (eV) Disp	Latt	Surf
X	PT	Si	Silicon	14	28	1	100.(	21	2.1	3.1

Special Parameters

Name of Calculation: Xe into Si/Pt/Si [Mixing a Marker]

Stopping Power Version: SRIM-2008

AutoSave at Ion #: 10000

Total Number of Ions: 999999

Random Number Seed:

Plotting Window Depths

Min: 0 Å

Max: 300 Å

Output Disk Files

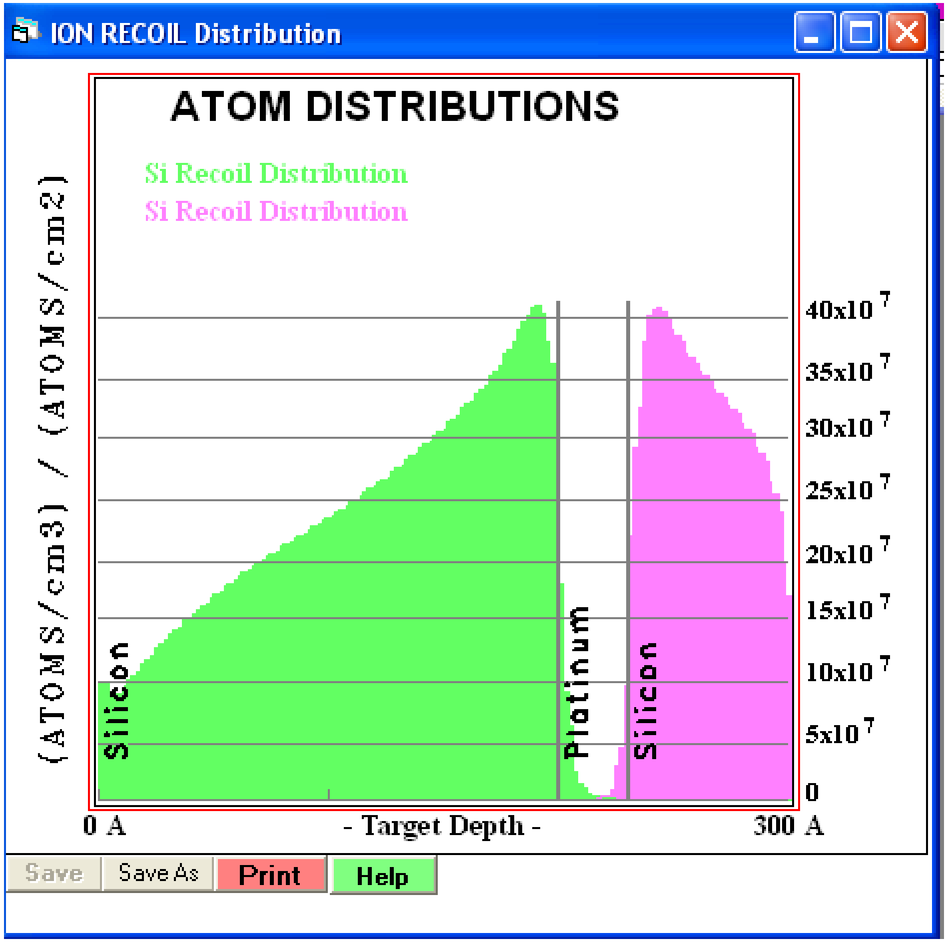
- ☐ Ion Ranges
- ☐ Backscattered Ions
- ☐ Transmitted Ions/Recoils
- ☐ Sputtered Atoms
- ☐ Collision Details

0 Special "EXYZ File" Increment (eV)

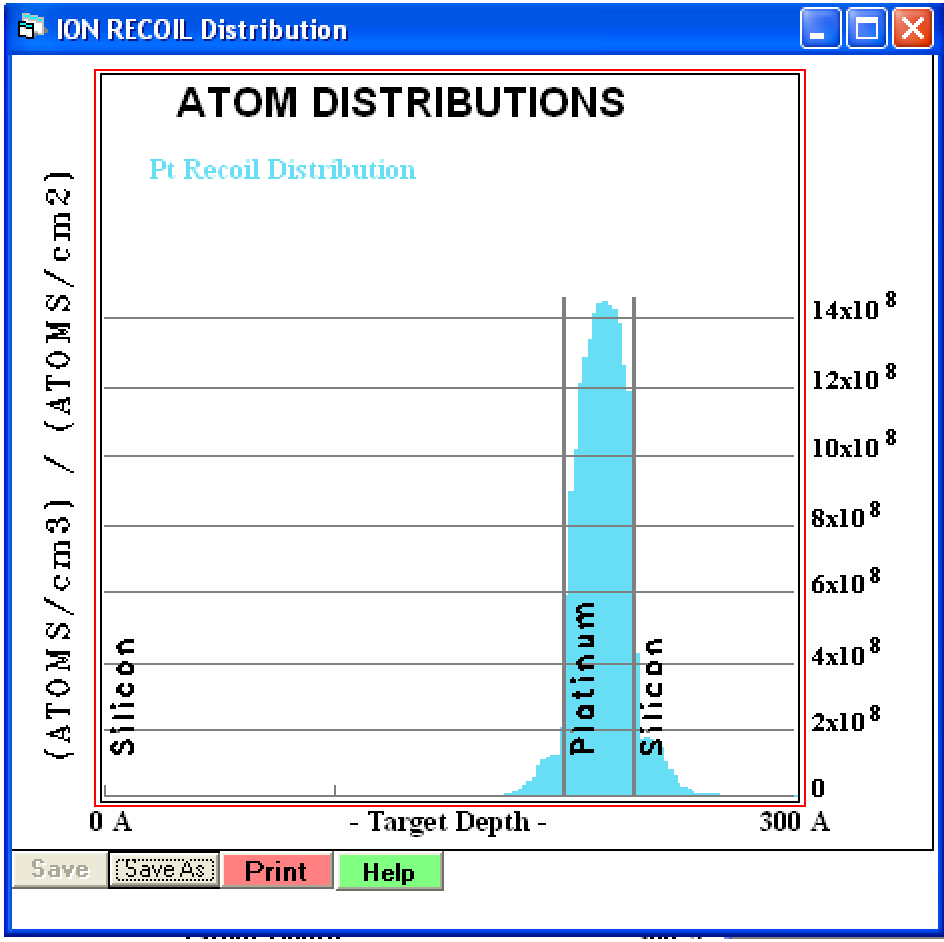
☐ Resume saved TRIM calc.

☐ Use TRIM-96 (DOS)

Distribution of Recoil Silicon

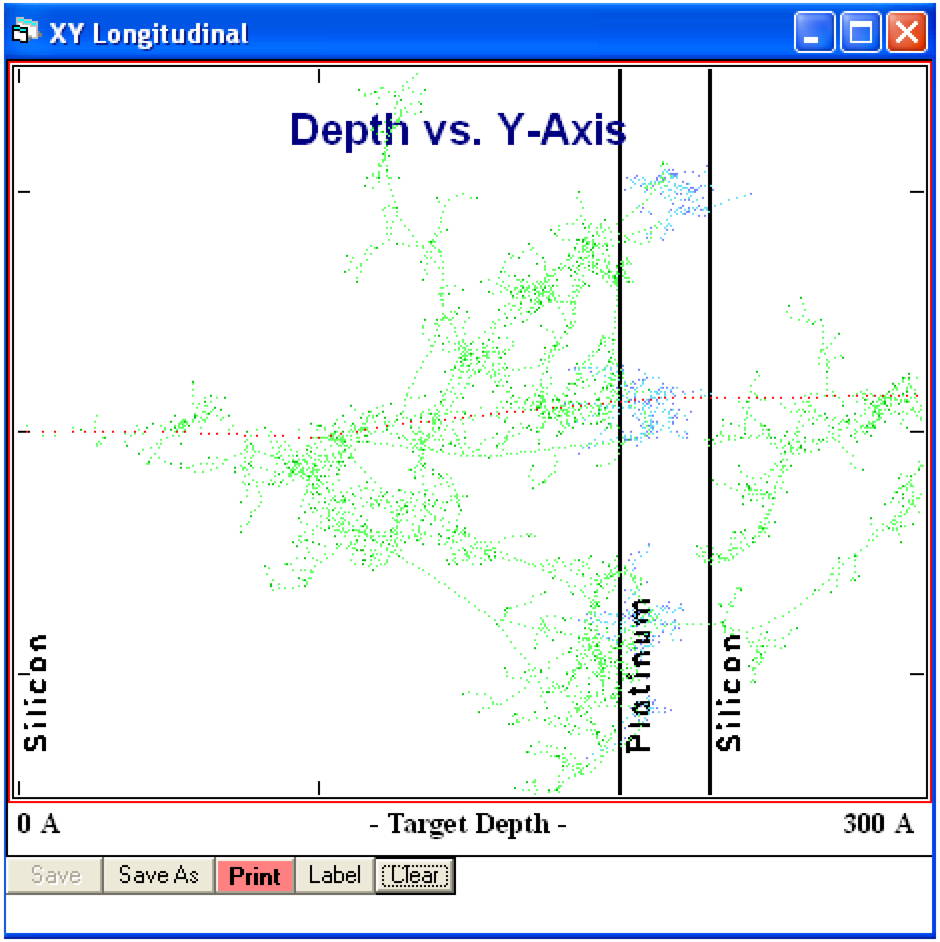


Distribution of Recoil Platinum

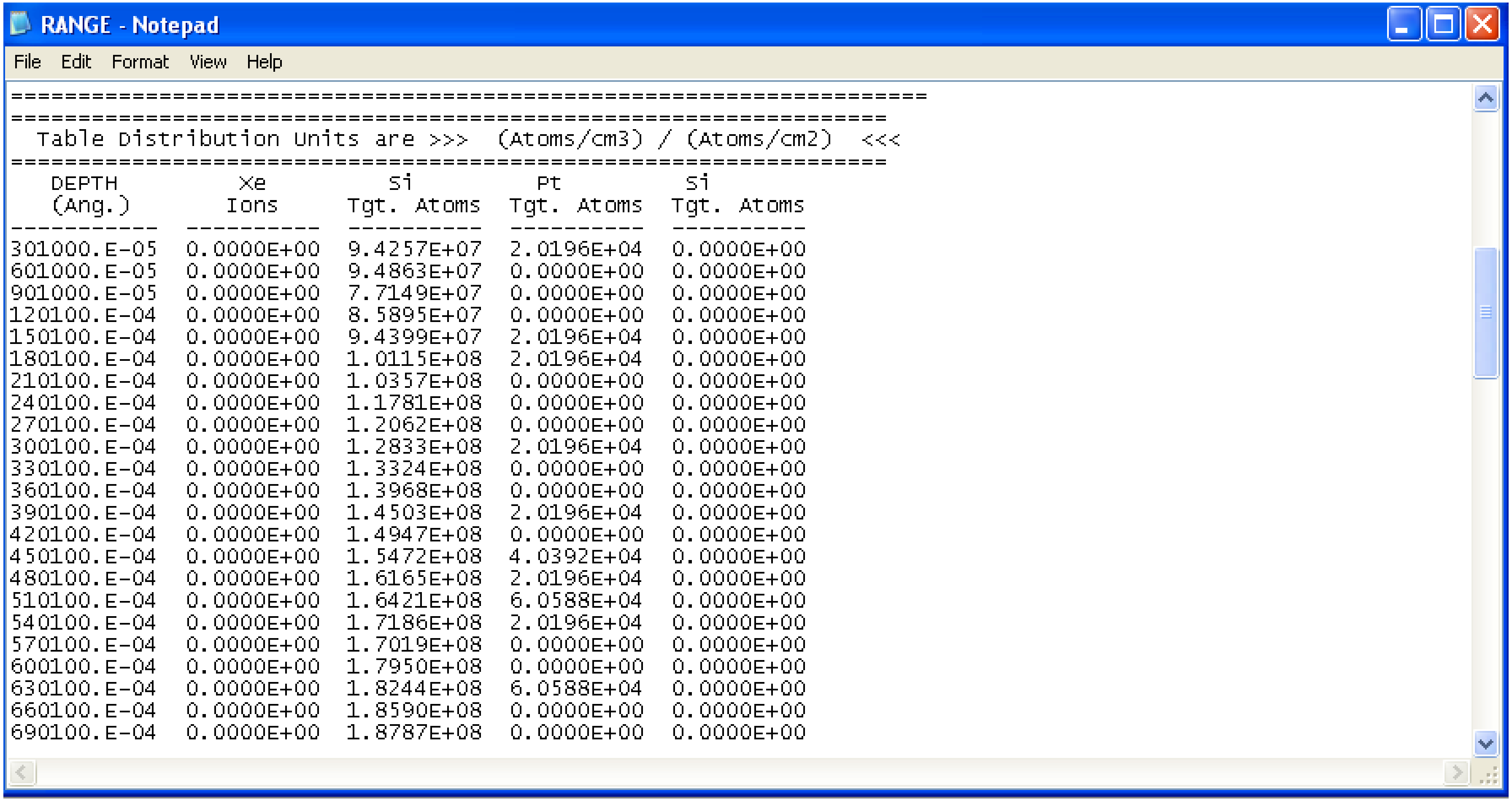


➢ Trajectory of Single Incidence Ion and Recoil Atoms

The big cascades rapidly lose any forward direction and become isotropic.



➢ Distribution of Recoil Platinum Atoms



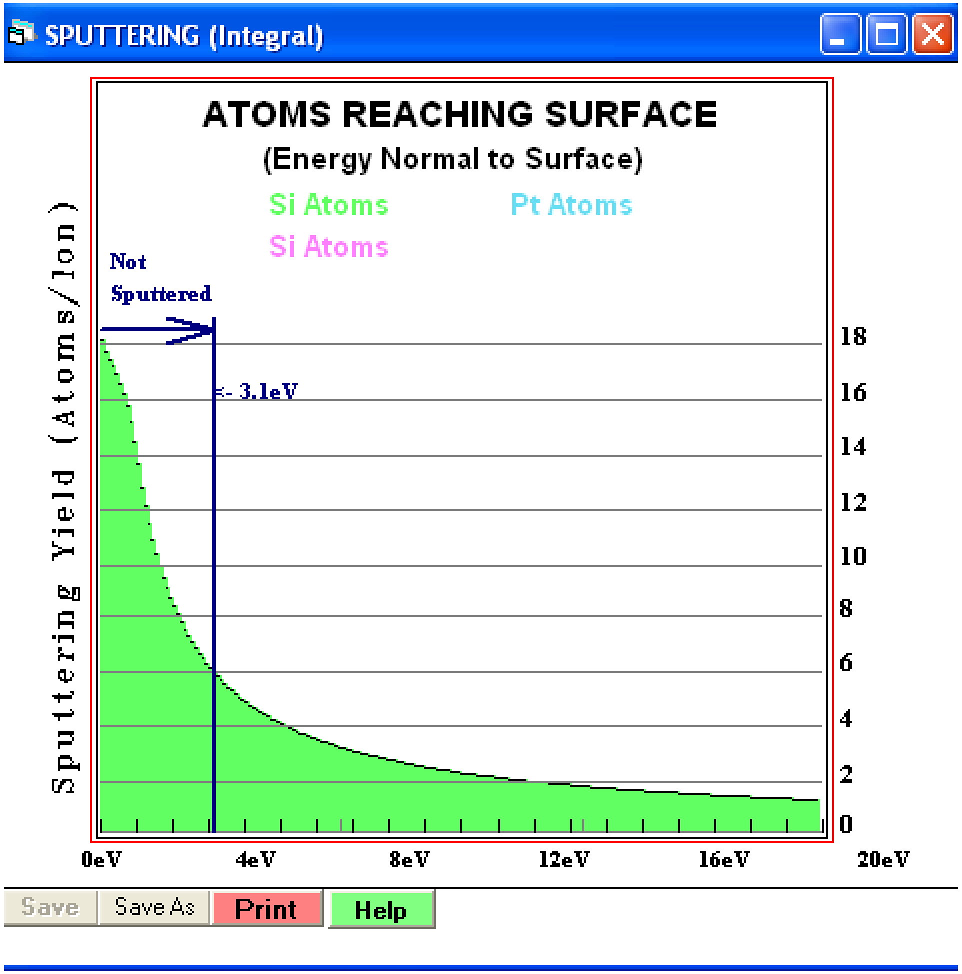
```
=====================================================================
==================================================================
  Table Distribution Units are >>>  (Atoms/cm3) / (Atoms/cm2)  <<<
==================================================================
   DEPTH         Xe          Si          Pt          Si
   (Ang.)       Ions     Tgt. Atoms  Tgt. Atoms  Tgt. Atoms
-----------  ----------  ----------  ----------  ----------
301000.E-05  0.0000E+00  9.4257E+07  2.0196E+04  0.0000E+00
601000.E-05  0.0000E+00  9.4863E+07  0.0000E+00  0.0000E+00
901000.E-05  0.0000E+00  7.7149E+07  0.0000E+00  0.0000E+00
120100.E-04  0.0000E+00  8.5895E+07  0.0000E+00  0.0000E+00
150100.E-04  0.0000E+00  9.4399E+07  2.0196E+04  0.0000E+00
180100.E-04  0.0000E+00  1.0115E+08  2.0196E+04  0.0000E+00
210100.E-04  0.0000E+00  1.0357E+08  0.0000E+00  0.0000E+00
240100.E-04  0.0000E+00  1.1781E+08  0.0000E+00  0.0000E+00
270100.E-04  0.0000E+00  1.2062E+08  0.0000E+00  0.0000E+00
300100.E-04  0.0000E+00  1.2833E+08  2.0196E+04  0.0000E+00
330100.E-04  0.0000E+00  1.3324E+08  0.0000E+00  0.0000E+00
360100.E-04  0.0000E+00  1.3968E+08  0.0000E+00  0.0000E+00
390100.E-04  0.0000E+00  1.4503E+08  2.0196E+04  0.0000E+00
420100.E-04  0.0000E+00  1.4947E+08  0.0000E+00  0.0000E+00
450100.E-04  0.0000E+00  1.5472E+08  4.0392E+04  0.0000E+00
480100.E-04  0.0000E+00  1.6165E+08  2.0196E+04  0.0000E+00
510100.E-04  0.0000E+00  1.6421E+08  6.0588E+04  0.0000E+00
540100.E-04  0.0000E+00  1.7186E+08  2.0196E+04  0.0000E+00
570100.E-04  0.0000E+00  1.7019E+08  0.0000E+00  0.0000E+00
600100.E-04  0.0000E+00  1.7950E+08  0.0000E+00  0.0000E+00
630100.E-04  0.0000E+00  1.8244E+08  6.0588E+04  0.0000E+00
660100.E-04  0.0000E+00  1.8590E+08  0.0000E+00  0.0000E+00
690100.E-04  0.0000E+00  1.8787E+08  0.0000E+00  0.0000E+00
```

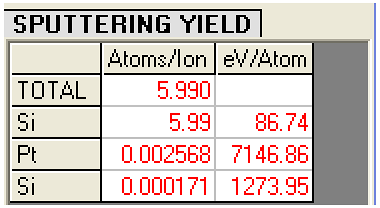
It shows that some Pt atoms have recoiled far back from the Pt layer – within 100 Å of the surface, and others have reached the back edge of the target.

➢ Sputtering yield (Integral)

The sputtering yield is very sensitive to the surface binding energy (SBE).

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.



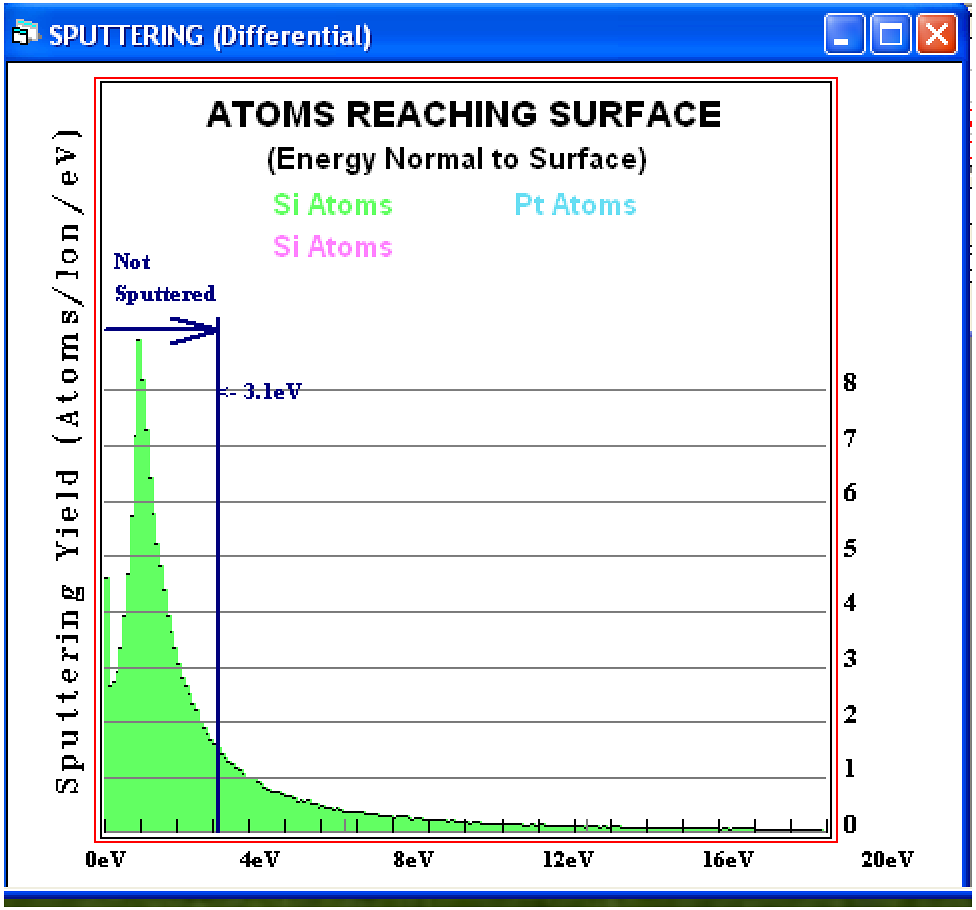


SPUTTERING YIELD

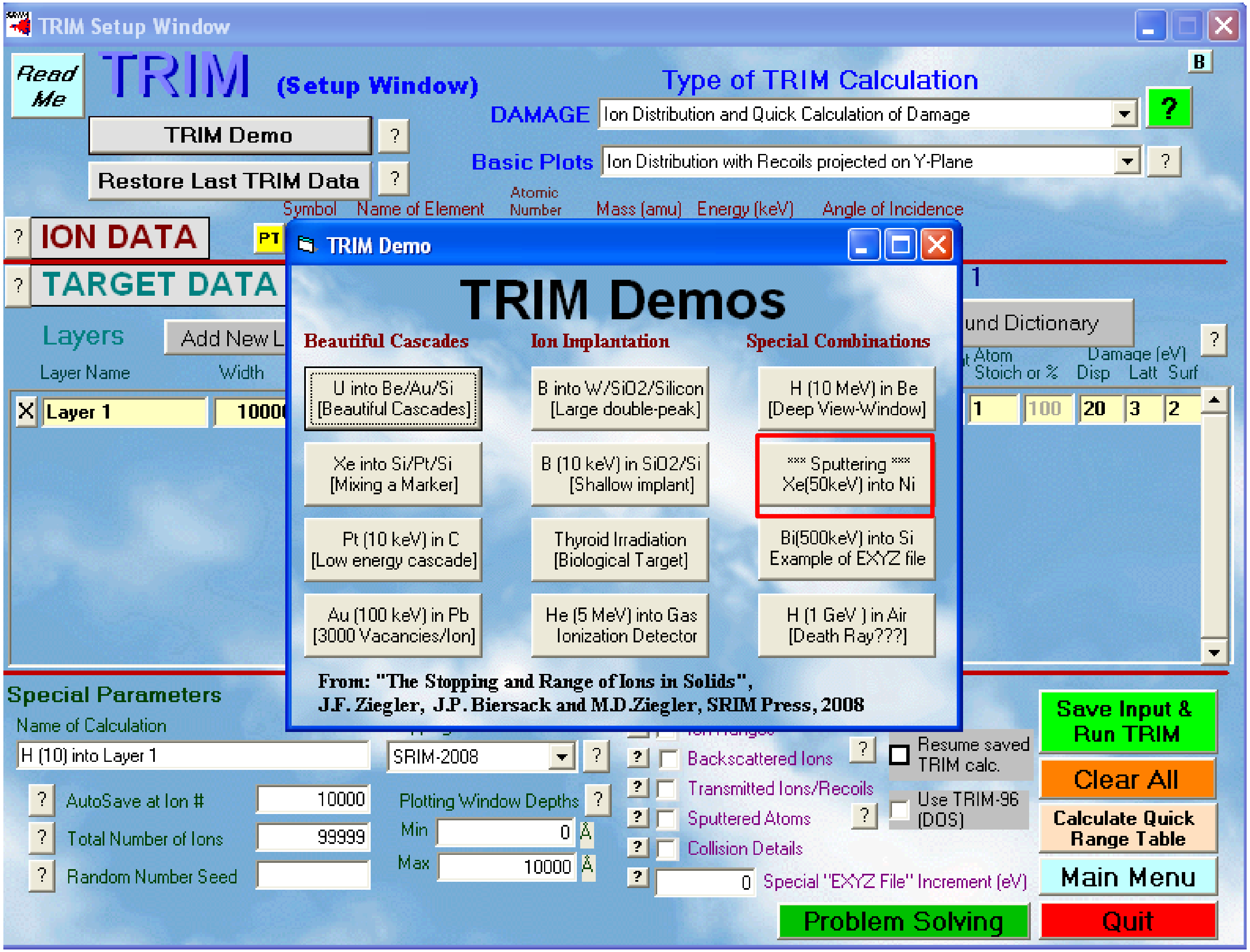
	Atoms/Ion	eV/Atom
TOTAL	5.990	
Si	5.99	86.74
Pt	0.002568	7146.86
Si	0.000171	1273.95

➢ Sputtering yield (Differential)

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.



➢ Extreme example of sputtering



DAMAGE: Ion Distribution and Quick Calculation of Damage

Basic Plots: Ion Distribution with Recoils projected on Y-Plane

Layer 1 | 10000 | 1 | 100 | 20 | 3 | 2

From: "The Stopping and Range of Ions in Solids",
J.F. Ziegler, J.P. Biersack and M.D.Ziegler, SRIM Press, 2008

Name of Calculation: H (10) into Layer 1

SRIM-2008

AutoSave at Ion #: 10000

Total Number of Ions: 99999

Random Number Seed:

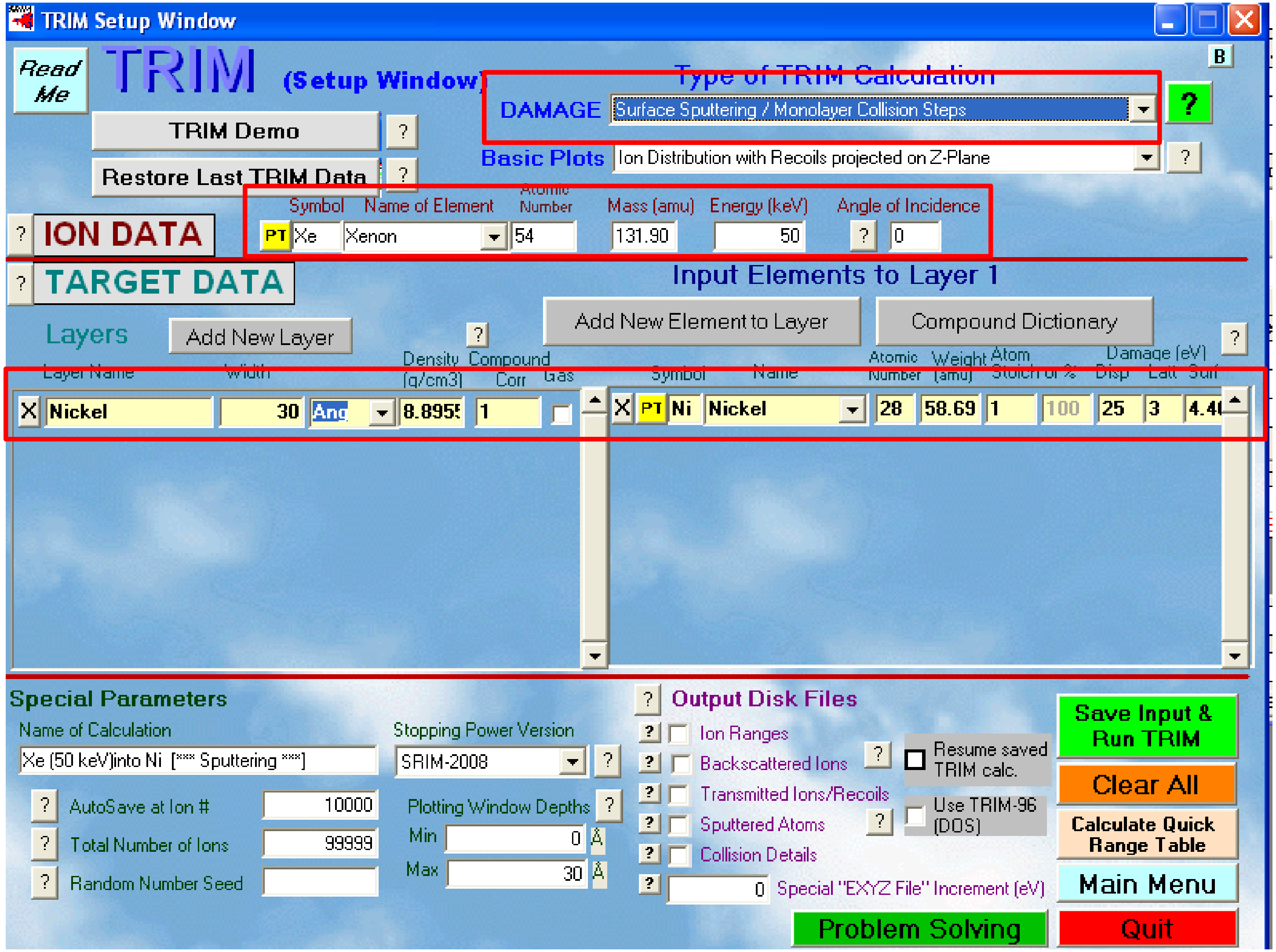
Plotting Window Depths: Min 0 Å, Max 10000 Å

Special "EXYZ File" Increment (eV): 0

SRIM Tutorials 2

➢ Extreme example of sputtering

Damage type:
Surface Sputtering.
Width: 30 Å



Type of TRIM Calculation: DAMAGE — Surface Sputtering / Monolayer Collision Steps

Basic Plots: Ion Distribution with Recoils projected on Z-Plane

Symbol	Name of Element	Atomic Number	Mass (amu)	Energy (keV)	Angle of Incidence
Xe	Xenon	54	131.90	50	0

Layer Name	Width		Density (g/cm3)	Compound Corr	Gas
Nickel	30	Ang	8.895	1	☐

Symbol	Name	Atomic Number	Weight (amu)	Atom Stoich	or %	Damage (eV) Disp	Latt	Surf
Ni	Nickel	28	58.69	1	100	25	3	4.4

Name of Calculation: Xe (50 keV)into Ni [*** Sputtering ***]

Stopping Power Version: SRIM-2008

AutoSave at Ion #: 10000

Total Number of Ions: 99999

Random Number Seed:

Plotting Window Depths: Min 0 Å, Max 30 Å

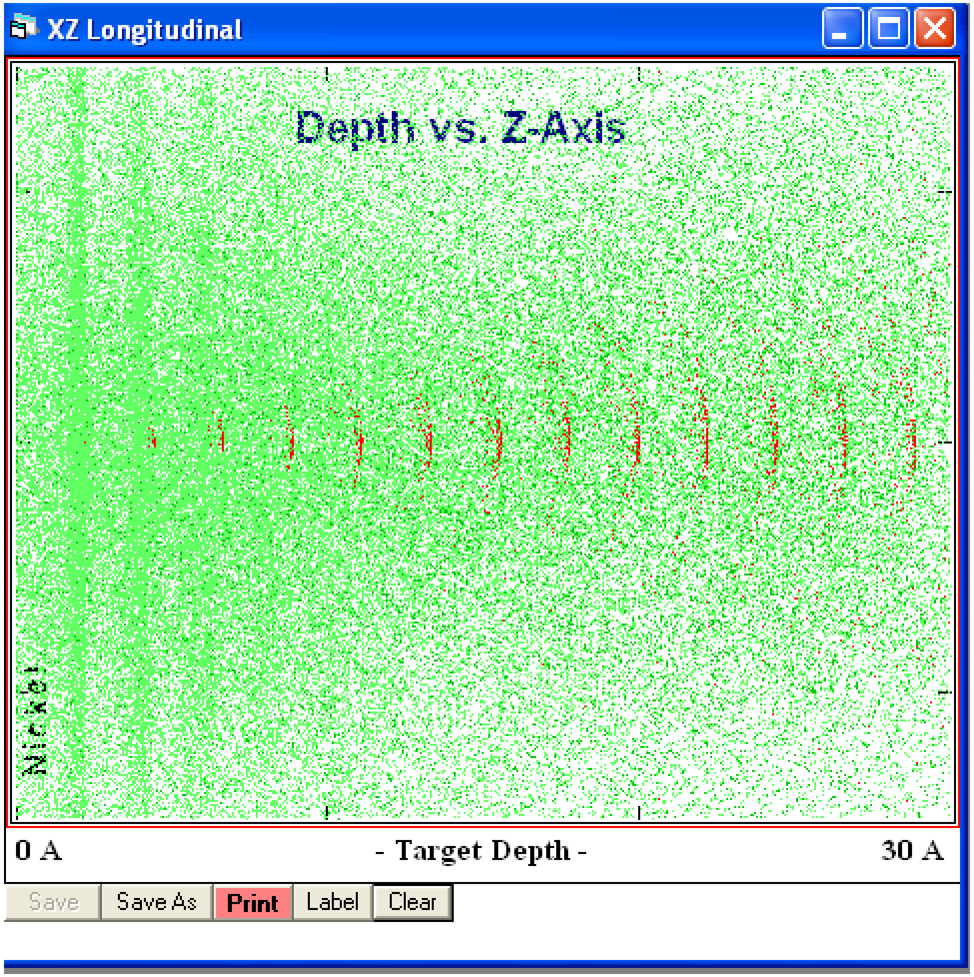
Output Disk Files:
- ☐ Ion Ranges
- ☐ Backscattered Ions
- ☐ Transmitted Ions/Recoils
- ☐ Sputtered Atoms
- ☐ Collision Details
- 0 Special "EXYZ File" Increment (eV)

☐ Resume saved TRIM calc.

☐ Use TRIM-96 (DOS)

➢ Extreme example of sputtering

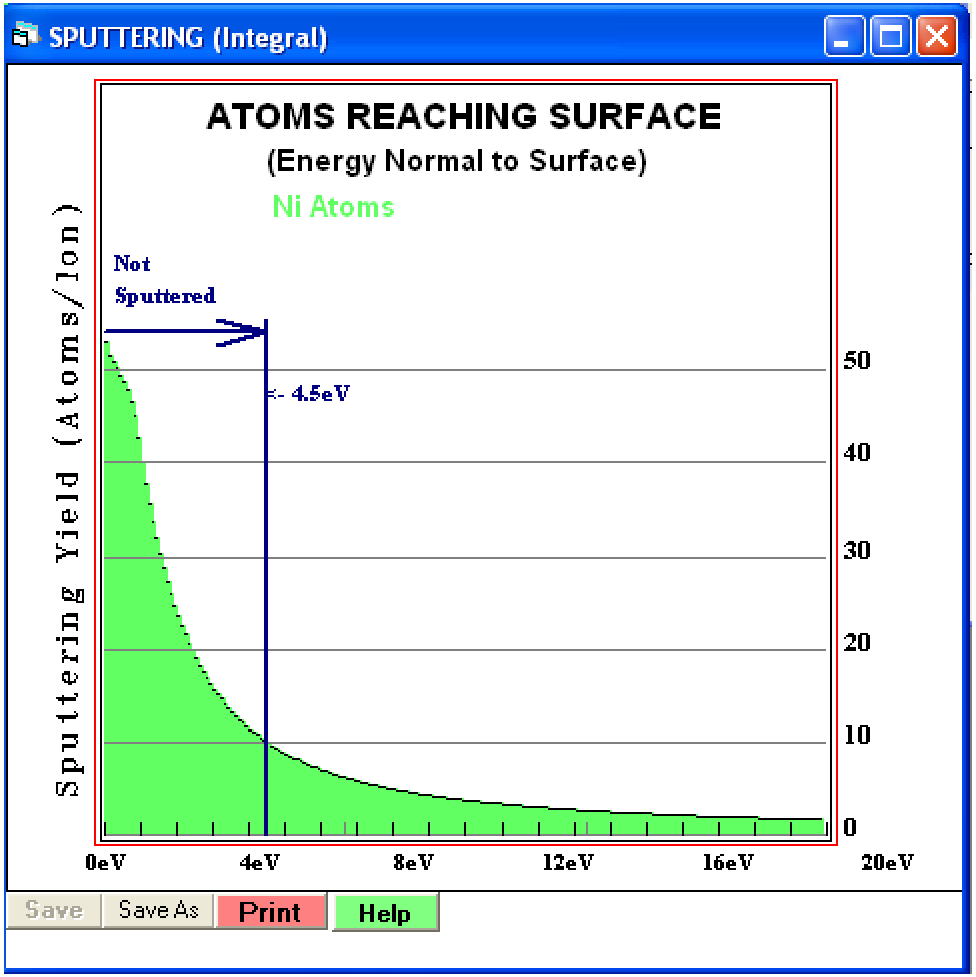
The spacing between atoms in Nickel is slightly more than 2 Angstroms, and this is the separation between the groups of crescent red dots.



SRIM Tutorials 2

➢ Extreme example of sputtering

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.



SUMMARY

- Interface Mixing can be a large effect with atoms moving more than 100 Å 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 Å below the surface.

Review

- **Tutorial 1: Introduction to Ion Ranges, Does and Damage**
  1. How to find the energy and dose of ions required to implant atoms into a target at given depth and concentration?
  2. How to calculate the damage deposited to target which was produced by the ion? Will the target be amorphous after the implant?
  3. How to use the SR table to quickly get the range of ions with different incident energy?
  4. How to setup the TRIM based on experimental parameters?

- **Tutorial 2: Target Mixing and Sputtering**
  1. The interface mixing, recoil implantation, sputtering yield.
  2. The importance of recoil cascade to interface and sputtering.
  3. The closed relationship between sputtering yield and surface binding energy.

Outline

Tutorial 1:
Introduction to Ion Ranges, Does and Damage

Tutorial 2:
Target Mixing and Sputtering

Tutorial 3:
Building Complex Targets

Tutorial 4:
Calculations of Target Damage

SRIM Tutorials 3: Building Complex Targets

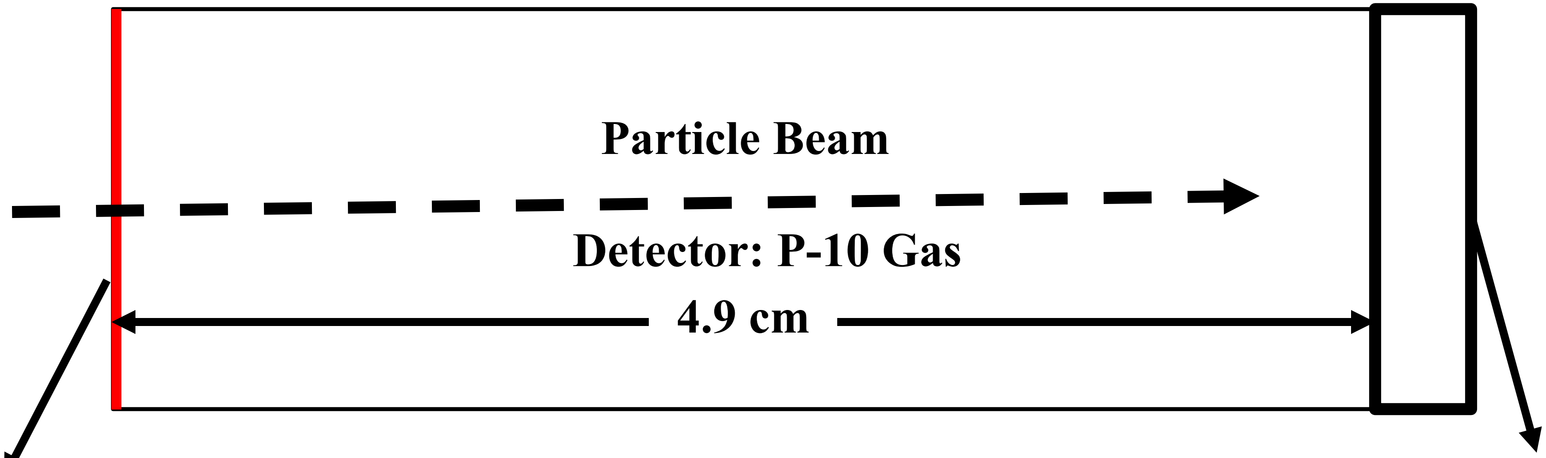
➢ Objective

To build a complex target: a Gas Ionization Detector for energetic ions with both Gas and Solid volumes.

➢ Case

To simulate a Gas Ionization Detector.

➢ Parameters



Particle Beam

Detector: P-10 Gas

4.9 cm

Thin Entrance Window:
1 μm Paralene “C”

Beam Stop:
2.5 mm Brass

SRIM Tutorials 3

➢ TRIM setup

◆ **Ion Data:**

1. **Ion species: Helium**
2. **Incident energy: 5 MeV (5000 keV)**
3. **Angle of incidence: normal (0°)**

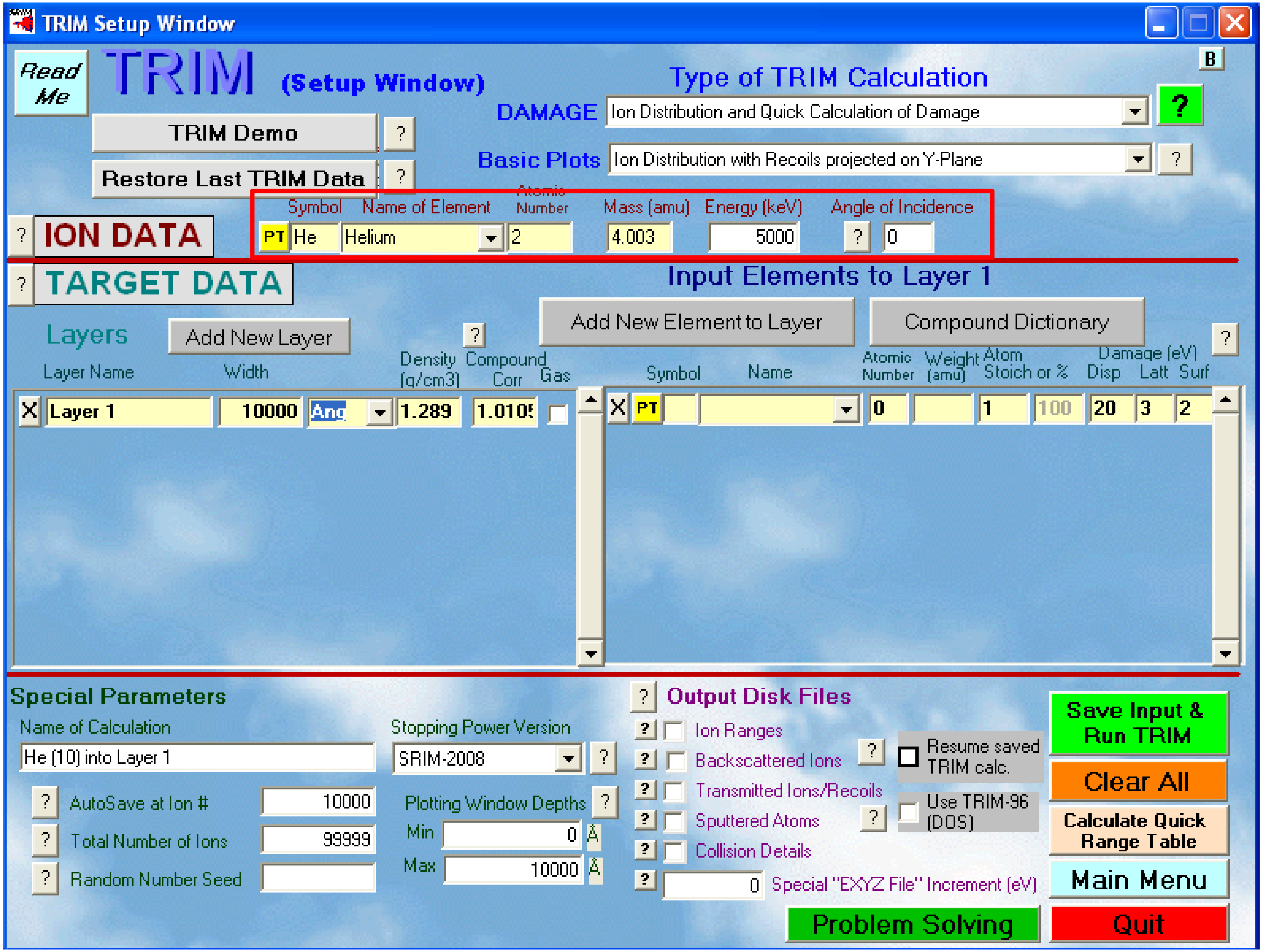
◆ **Target Data:**

Three layers complex target.

1. **Surface thin film: Paralene “C”, 1 μm**
2. **Long cylinder of gas: P-10 gas(10%CH_4 and 90% Ar), 4.9 cm**
3. **Brass beam stop: brass, 2.5mm**

➢ TRIM setup

Ion Data



Type of TRIM Calculation

DAMAGE: Ion Distribution and Quick Calculation of Damage

Basic Plots: Ion Distribution with Recoils projected on Y-Plane

Symbol	Name of Element	Atomic Number	Mass (amu)	Energy (keV)	Angle of Incidence
He	Helium	2	4.003	5000	0

Layers

Layer Name	Width		Density (g/cm3)	Compound Corr	Gas
Layer 1	10000	Ang	1.289	1.010	☐

Input Elements to Layer 1

Symbol	Name	Atomic Number	Weight (amu)	Atom Stoich	or %	Damage (eV) Disp	Latt	Surf
		0		1	100	20	3	2

Special Parameters

Name of Calculation: He (10) into Layer 1

Stopping Power Version: SRIM-2008

AutoSave at Ion #: 10000

Total Number of Ions: 99999

Random Number Seed:

Plotting Window Depths: Min 0 Å, Max 10000 Å

Output Disk Files

☐ Ion Ranges

☐ Backscattered Ions

☐ Transmitted Ions/Recoils

☐ Sputtered Atoms

☐ Collision Details

0 Special "EXYZ File" Increment (eV)

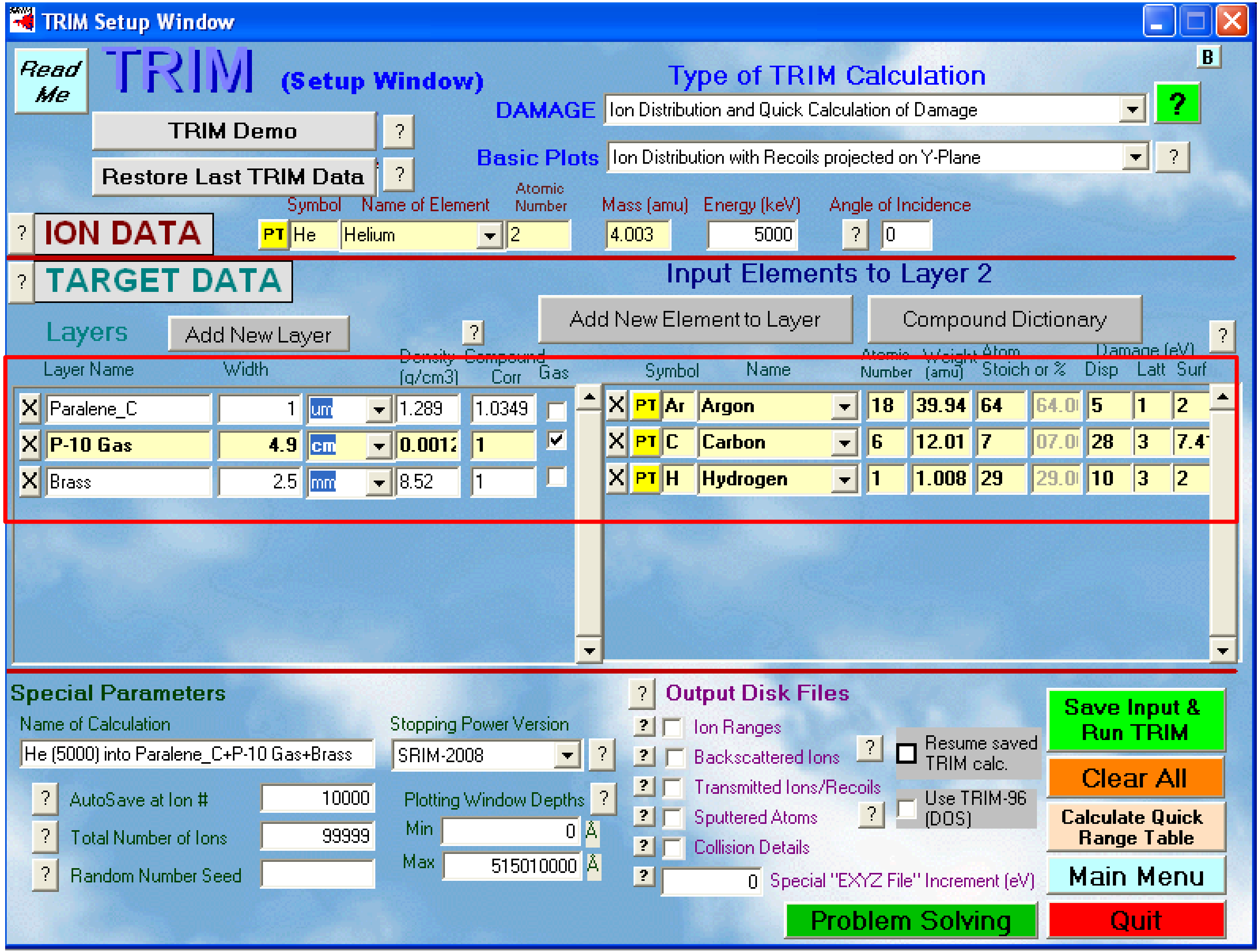
☐ Resume saved TRIM calc.

☐ Use TRIM-96 (DOS)

SRIM Tutorials 3

- **TRIM setup**

Target Data



Type of TRIM Calculation

DAMAGE: Ion Distribution and Quick Calculation of Damage

Basic Plots: Ion Distribution with Recoils projected on Y-Plane

ION DATA

Symbol	Name of Element	Atomic Number	Mass (amu)	Energy (keV)	Angle of Incidence
PT He	Helium	2	4.003	5000	0

TARGET DATA

Layers

	Layer Name	Width		Density (g/cm3)	Compound Corr	Gas
X	Paralene_C	1	um	1.289	1.0349	☐
X	P-10 Gas	4.9	cm	0.0012	1	☑
X	Brass	2.5	mm	8.52	1	☐

Input Elements to Layer 2

		Symbol	Name	Atomic Number	Weight (amu)	Atom Stoich or %		Damage (eV) Disp	Latt	Surf
X	PT	Ar	Argon	18	39.94	64	64.0	5	1	2
X	PT	C	Carbon	6	12.01	7	07.0	28	3	7.41
X	PT	H	Hydrogen	1	1.008	29	29.0	10	3	2

Special Parameters

Name of Calculation: He (5000) into Paralene_C+P-10 Gas+Brass

Stopping Power Version: SRIM-2008

AutoSave at Ion #: 10000

Total Number of Ions: 99999

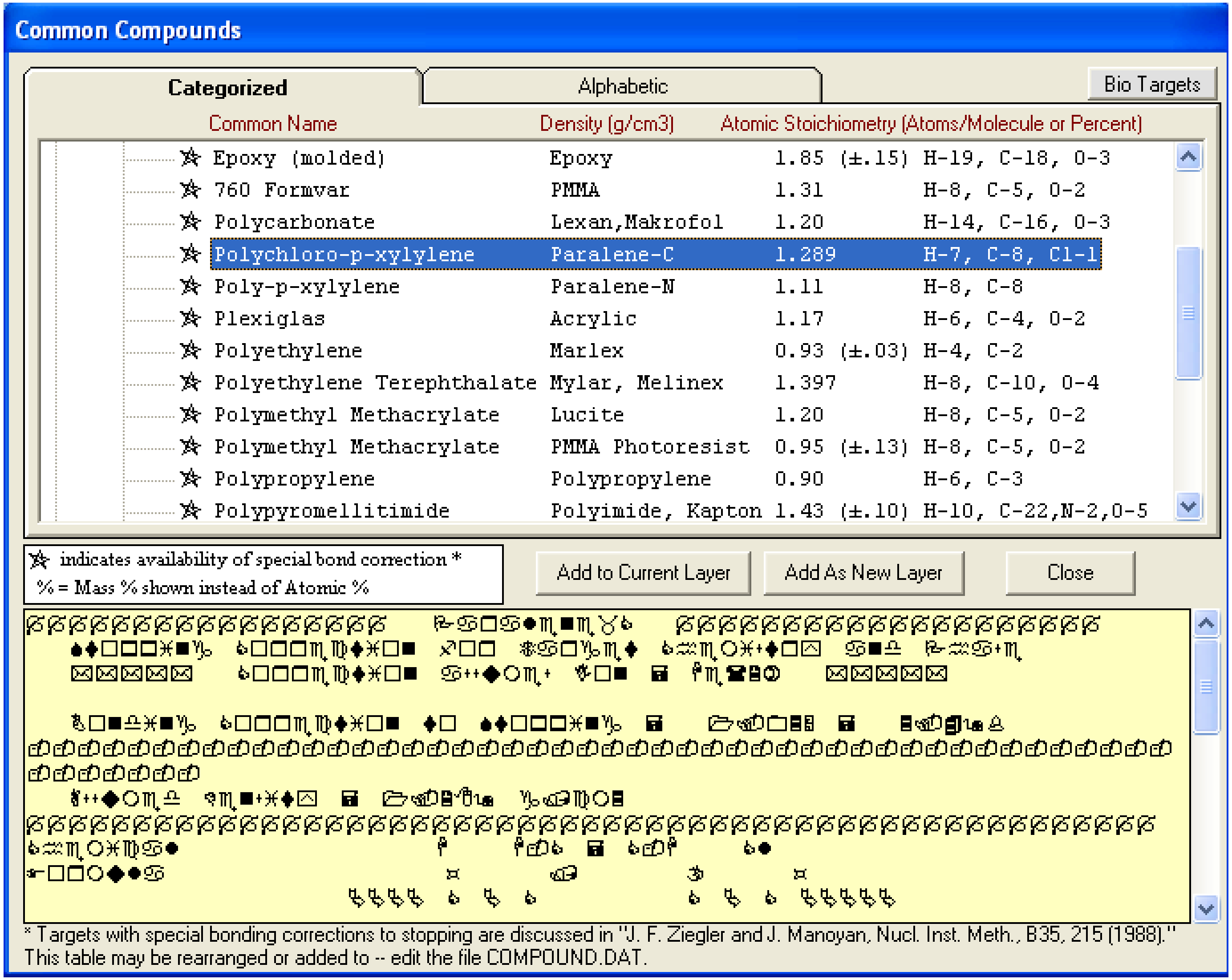
Random Number Seed:

Plotting Window Depths
Min: 0 Å
Max: 515010000 Å

Output Disk Files

☐ Ion Ranges
☐ Backscattered Ions
☐ Transmitted Ions/Recoils
☐ Sputtered Atoms
☐ Collision Details
0 Special "EXYZ File" Increment (eV)

☐ Resume saved TRIM calc.
☐ Use TRIM-96 (DOS)



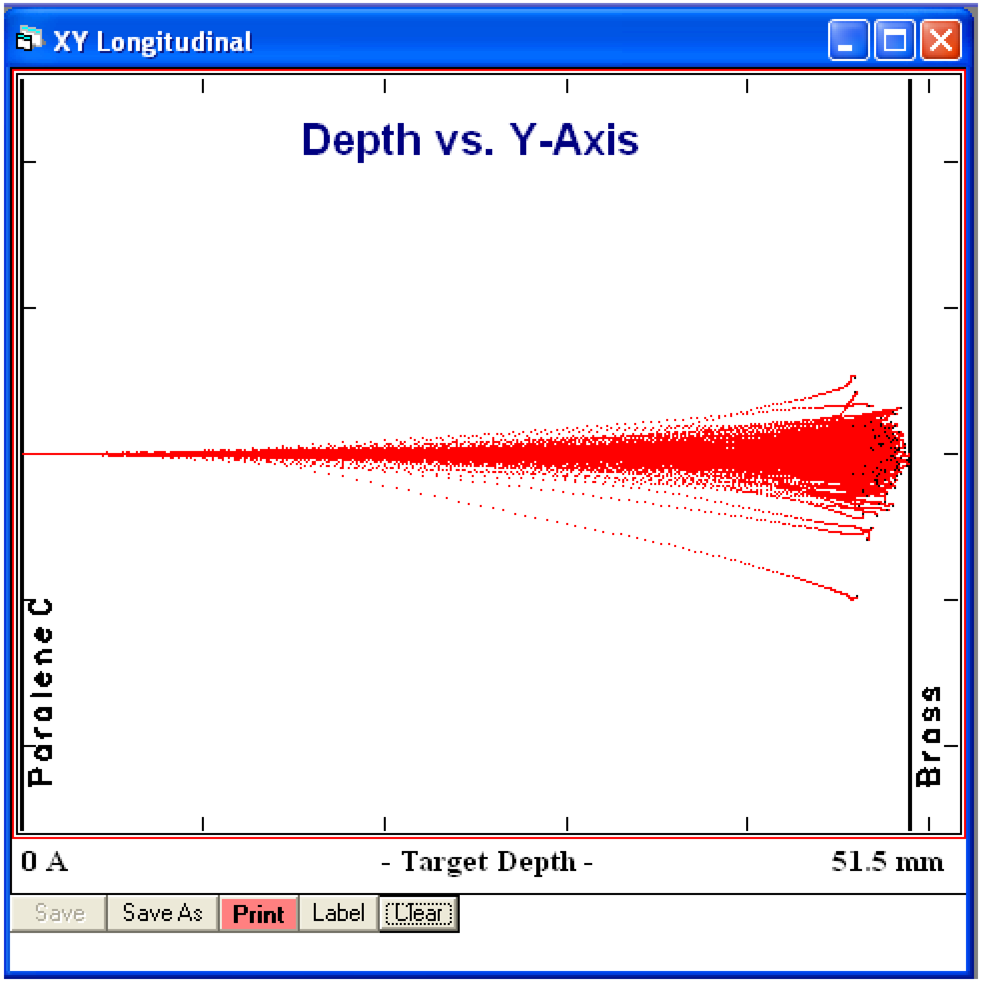
Common Compounds

Common Name		Density (g/cm3)	Atomic Stoichiometry (Atoms/Molecule or Percent)
☆ Epoxy (molded)	Epoxy	1.85 (±.15)	H-19, C-18, O-3
☆ 760 Formvar	PMMA	1.31	H-8, C-5, O-2
☆ Polycarbonate	Lexan,Makrofol	1.20	H-14, C-16, O-3
☆ Polychloro-p-xylylene	Paralene-C	1.289	H-7, C-8, Cl-1
☆ Poly-p-xylylene	Paralene-N	1.11	H-8, C-8
☆ Plexiglas	Acrylic	1.17	H-6, C-4, O-2
☆ Polyethylene	Marlex	0.93 (±.03)	H-4, C-2
☆ Polyethylene Terephthalate	Mylar, Melinex	1.397	H-8, C-10, O-4
☆ Polymethyl Methacrylate	Lucite	1.20	H-8, C-5, O-2
☆ Polymethyl Methacrylate	PMMA Photoresist	0.95 (±.13)	H-8, C-5, O-2
☆ Polypropylene	Polypropylene	0.90	H-6, C-3
☆ Polypyromellitimide	Polyimide, Kapton	1.43 (±.10)	H-10, C-22,N-2,O-5

☆ indicates availability of special bond correction *
% = Mass % shown instead of Atomic %

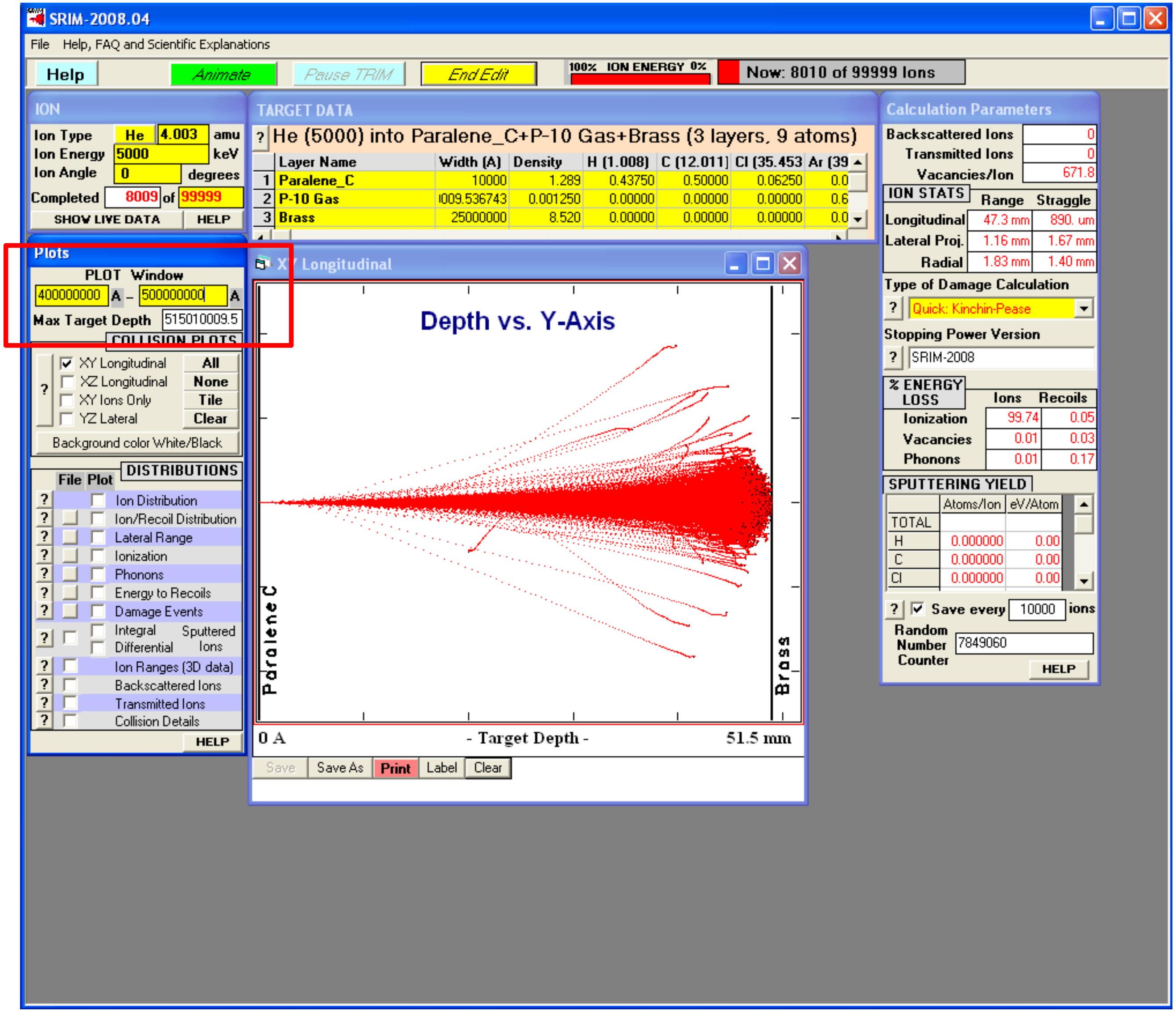
* Targets with special bonding corrections to stopping are discussed in "J. F. Ziegler and J. Manoyan, Nucl. Inst. Meth., B35, 215 (1988)."
This table may be rearranged or added to -- edit the file COMPOUND.DAT.

➢ Trajectories of ions



SRIM Tutorials 3

➢ Change range



Now: 8010 of 99999 Ions

Ion Type: He, 4.003 amu
Ion Energy: 5000 keV
Ion Angle: 0 degrees
Completed: 8009 of 99999

PLOT Window

400000000 A – 500000000 A

Max Target Depth: 515010009.5

COLLISION PLOTS

- ☑ XY Longitudinal
- ☐ XZ Longitudinal
- ☐ XY Ions Only
- ☐ YZ Lateral

- ☐ Ion Distribution
- ☐ Ion/Recoil Distribution
- ☐ Lateral Range
- ☐ Ionization
- ☐ Phonons
- ☐ Energy to Recoils
- ☐ Damage Events
- ☐ Integral / ☐ Differential — Sputtered Ions
- ☐ Ion Ranges (3D data)
- ☐ Backscattered Ions
- ☐ Transmitted Ions
- ☐ Collision Details

TARGET DATA

He (5000) into Paralene_C+P-10 Gas+Brass (3 layers, 9 atoms)

	Layer Name	Width (A)	Density	H (1.008)	C (12.011)	Cl (35.453	Ar (39
1	Paralene_C	10000	1.289	0.43750	0.50000	0.06250	0.0
2	P-10 Gas	ı009.536743	0.001250	0.00000	0.00000	0.00000	0.6
3	Brass	25000000	8.520	0.00000	0.00000	0.00000	0.0

0 A - Target Depth - 51.5 mm

Backscattered Ions: 0
Transmitted Ions: 0
Vacancies/Ion: 671.8

ION STATS	Range	Straggle
Longitudinal	47.3 mm	890. um
Lateral Proj.	1.16 mm	1.67 mm
Radial	1.83 mm	1.40 mm

Type of Damage Calculation: Quick: Kinchin-Pease

Stopping Power Version: SRIM-2008

% ENERGY LOSS	Ions	Recoils
Ionization	99.74	0.05
Vacancies	0.01	0.03
Phonons	0.01	0.17

SPUTTERING YIELD

	Atoms/Ion	eV/Atom
TOTAL		
H	0.000000	0.00
C	0.000000	0.00
Cl	0.000000	0.00

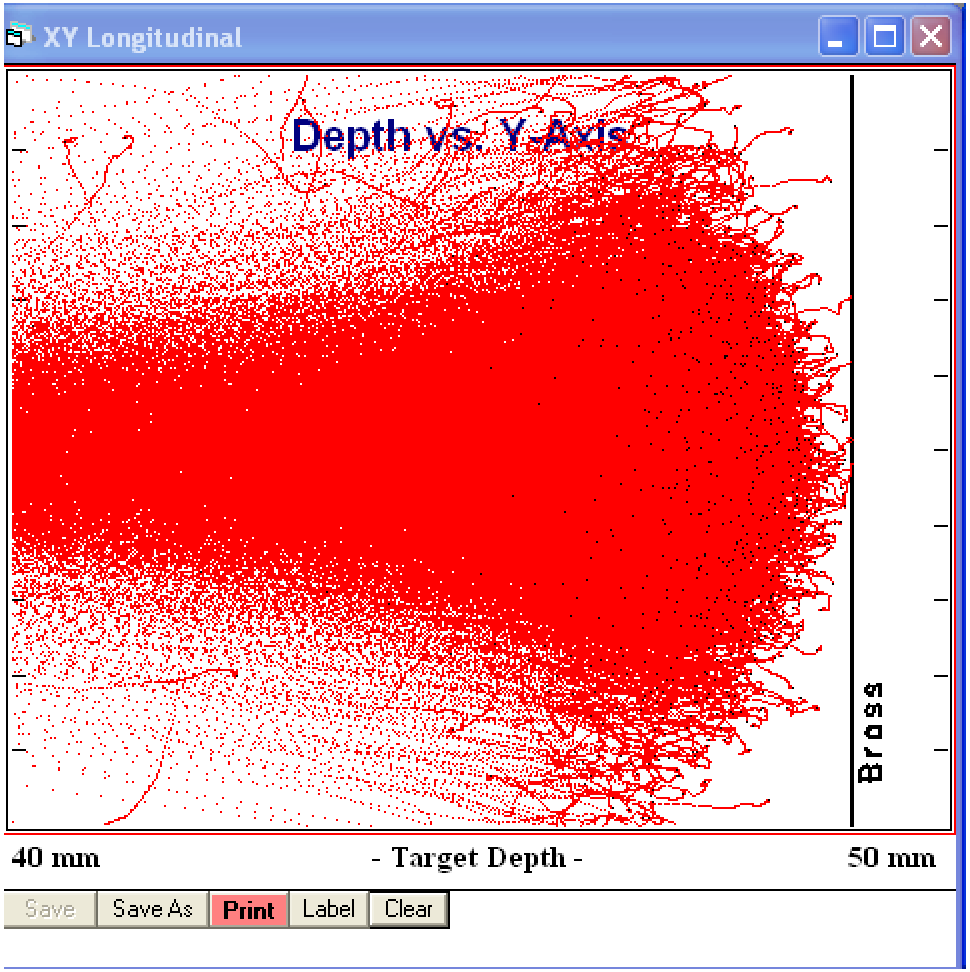
☑ Save every 10000 ions

Random Number Counter: 7849060

SRIM Tutorials 3

➢ End range of ions

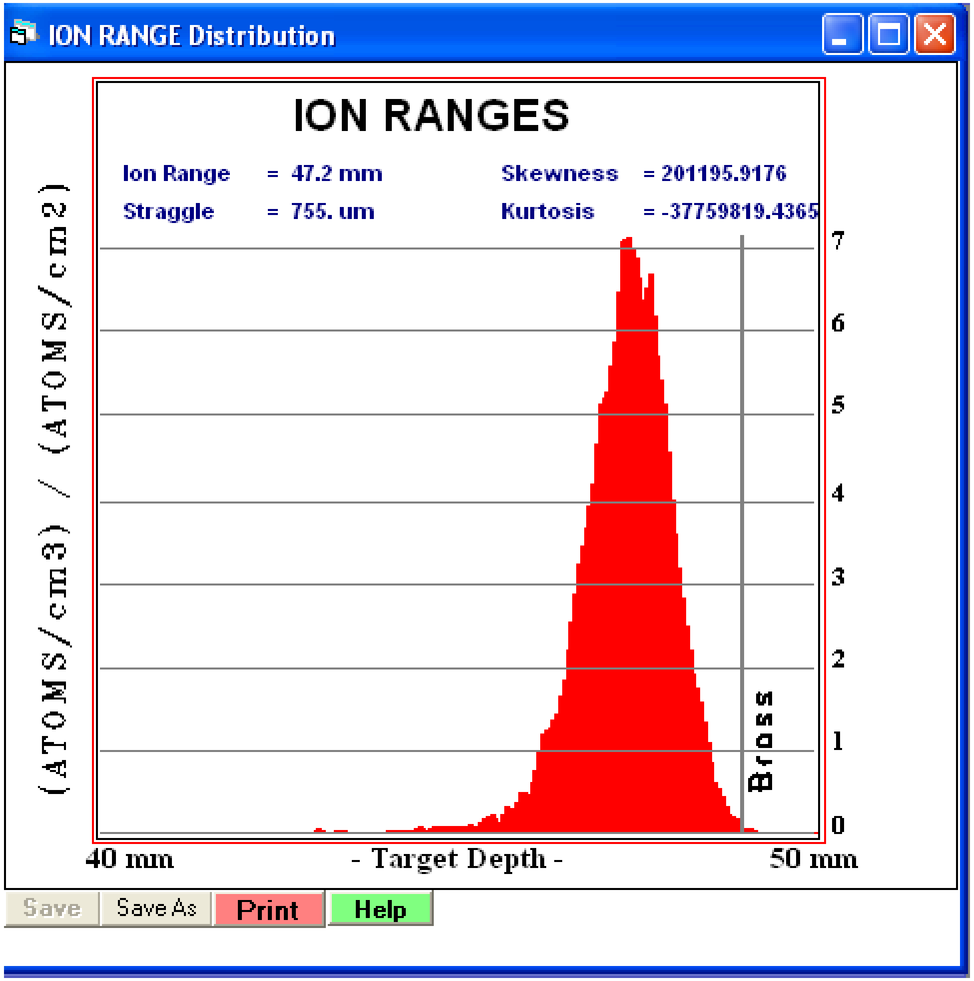
The He beam remains tightly focused until the He energy drops below 100 keV, or 2% of its original energy of 5 MeV.



SRIM Tutorials 3

Ion distribution

- Nice Gaussian shape
- Straggle only 2%



ION RANGE Distribution

ION RANGES

Ion Range = 47.2 mm

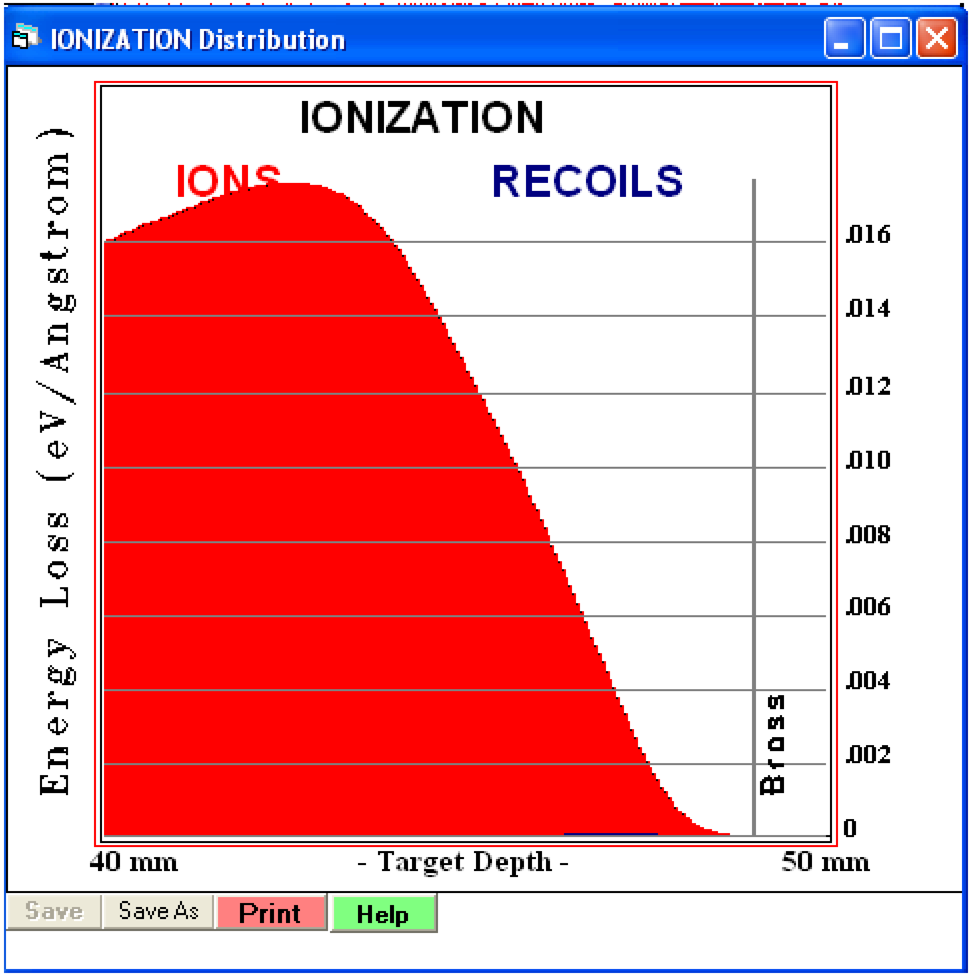
Straggle = 755. um

Skewness = 201195.9176

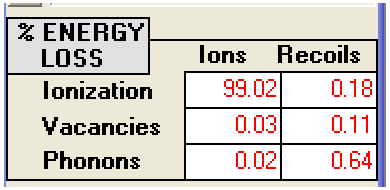
Kurtosis = -37759819.4365

SRIM Tutorials 3

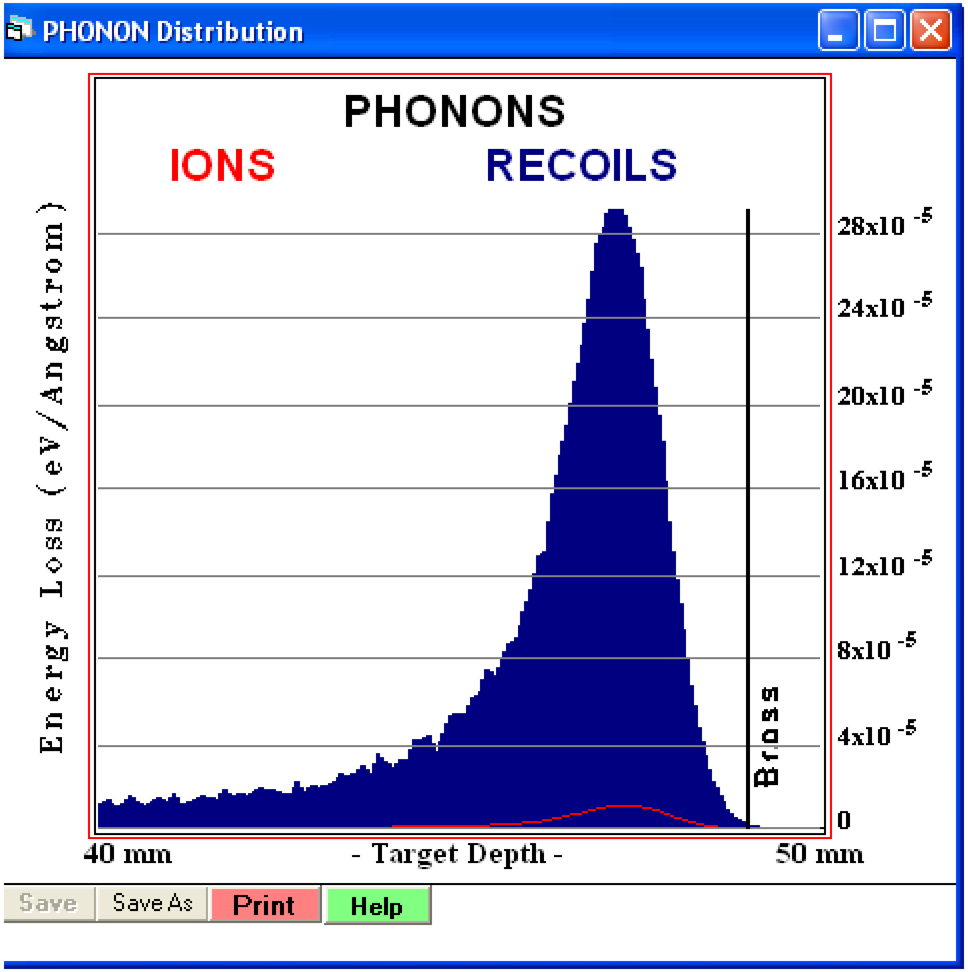
➢ Ionization



Phonons distribution



% ENERGY LOSS	Ions	Recoils
Ionization	99.02	0.18
Vacancies	0.03	0.11
Phonons	0.02	0.64



Outline

Tutorial 1:
Introduction to Ion Ranges, Does and Damage

Tutorial 2:
Target Mixing and Sputtering

Tutorial 3:
Building Complex Targets

Tutorial 4:
Calculations of Target Damage

SRIM Tutorials 4: Calculations of Target Damage

Objective

Detail calculate the target damage during implantation.

Case

Refer to tutorials 1.

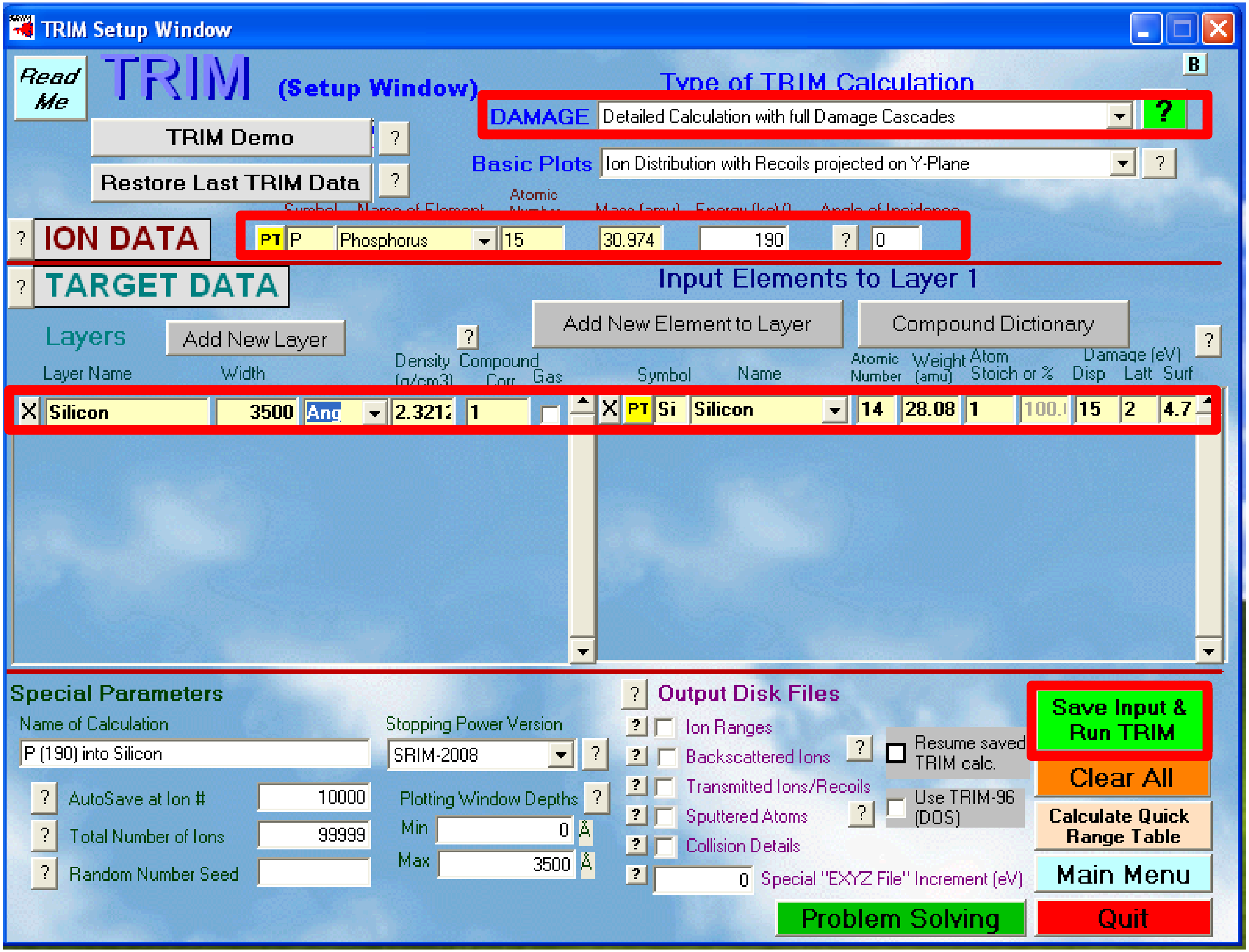
Parameters

Refer to tutorials 1.

Normally, implanting at room-temperature, 300 K, will cause most of the implantation damage to “self-anneal” since the lattice atoms have adequate energy to allow simple target damage to regrow back into its original crystalline form.

However, there are no thermal effects in SRIM, so the damage which is calculated is that which would happen for an implantation at 0 K.

TRIM setup



Type of TRIM Calculation

DAMAGE: Detailed Calculation with full Damage Cascades

Basic Plots: Ion Distribution with Recoils projected on Y-Plane

ION DATA

Symbol	Name of Element	Atomic Number	Mass (amu)	Energy (keV)	Angle of Incidence
P	Phosphorus	15	30.974	190	0

TARGET DATA

Layer Name	Width		Density (g/cm3)	Compound Corr	Gas
Silicon	3500	Ang	2.321	1	☐

Input Elements to Layer 1

Symbol	Name	Atomic Number	Weight (amu)	Atom Stoich	or %	Damage (eV) Disp	Latt	Surf
Si	Silicon	14	28.08	1	100.	15	2	4.7

Special Parameters

Name of Calculation: P (190) into Silicon

Stopping Power Version: SRIM-2008

AutoSave at Ion #: 10000

Total Number of Ions: 99999

Random Number Seed:

Plotting Window Depths: Min 0 Å, Max 3500 Å

Output Disk Files

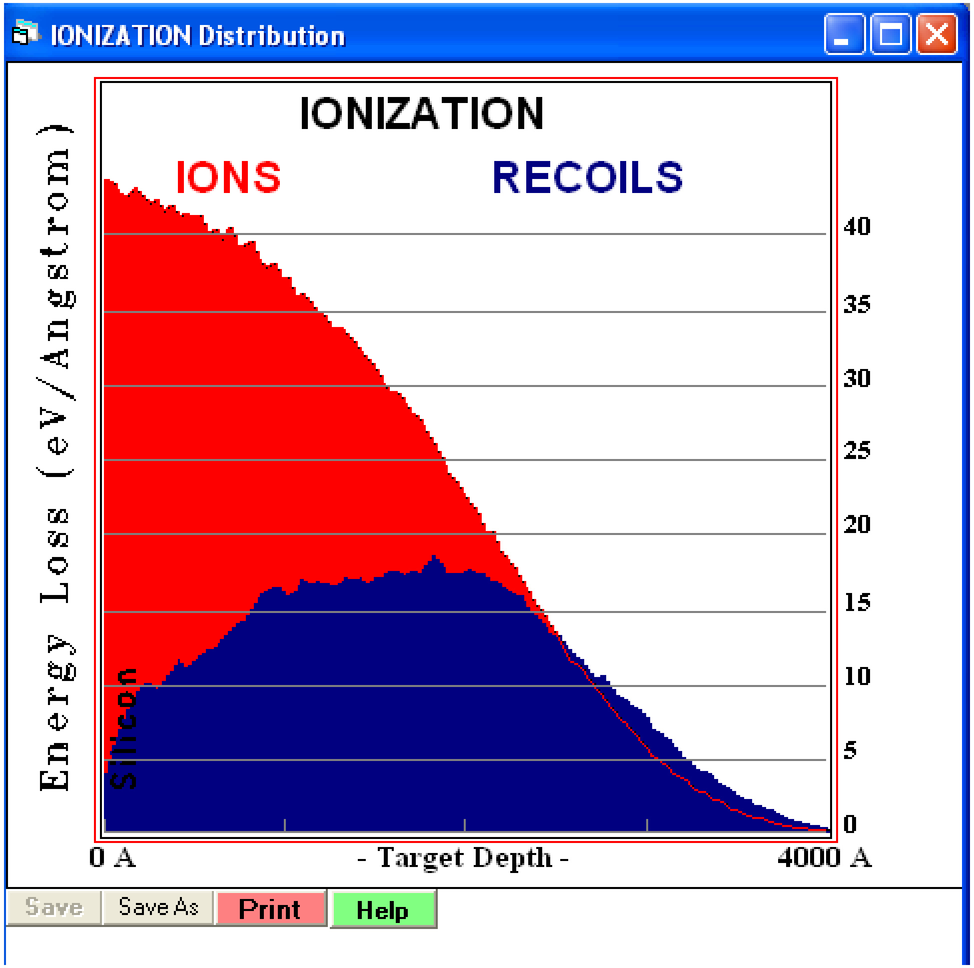
- ☐ Ion Ranges
- ☐ Backscattered Ions
- ☐ Transmitted Ions/Recoils
- ☐ Sputtered Atoms
- ☐ Collision Details
- 0 Special "EXYZ File" Increment (eV)

☐ Resume saved TRIM calc.

☐ Use TRIM-96 (DOS)

➢ Ionization

Ionization is energy loss to the target electrons.

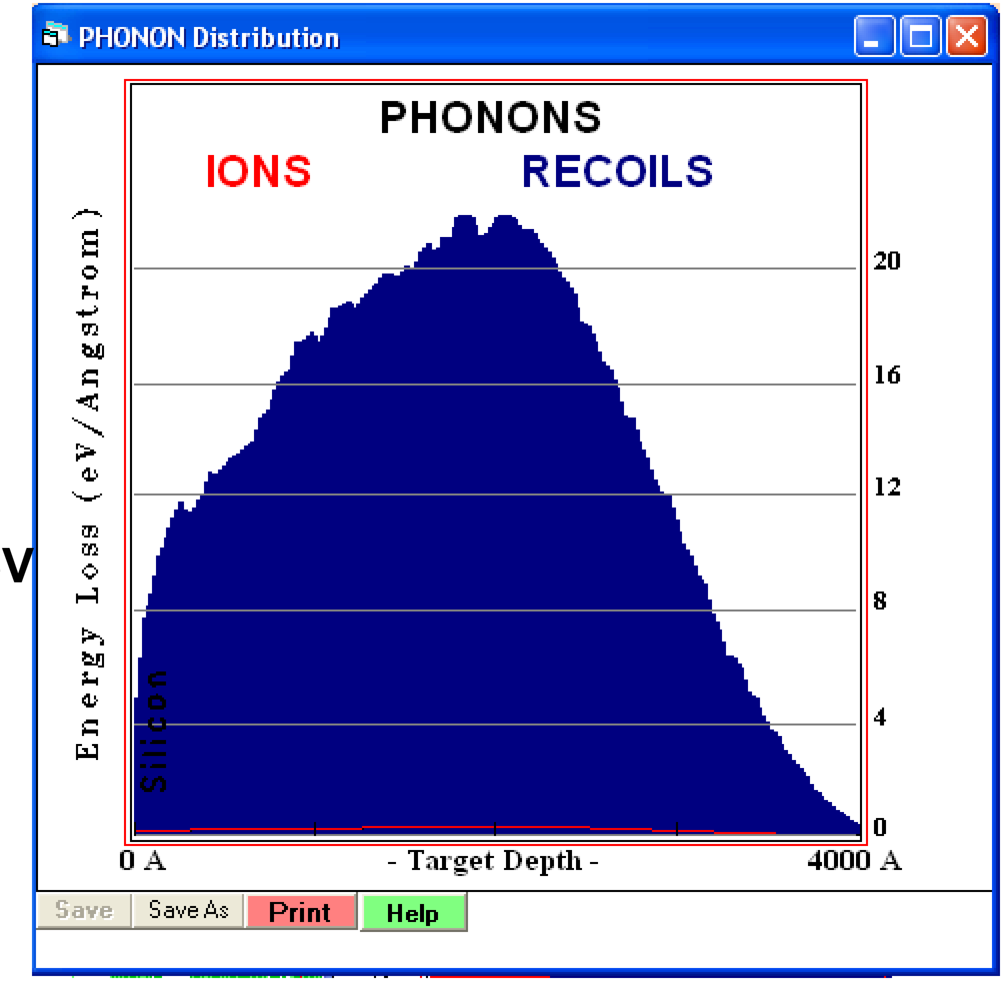


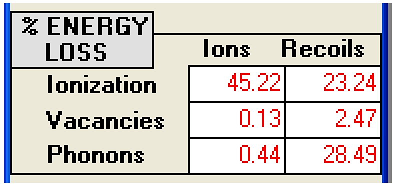
➢ Phonons

Phonons are energy stored in atomic vibrations in a crystal.

Ion: 190 keV x 0.44% = 836 eV

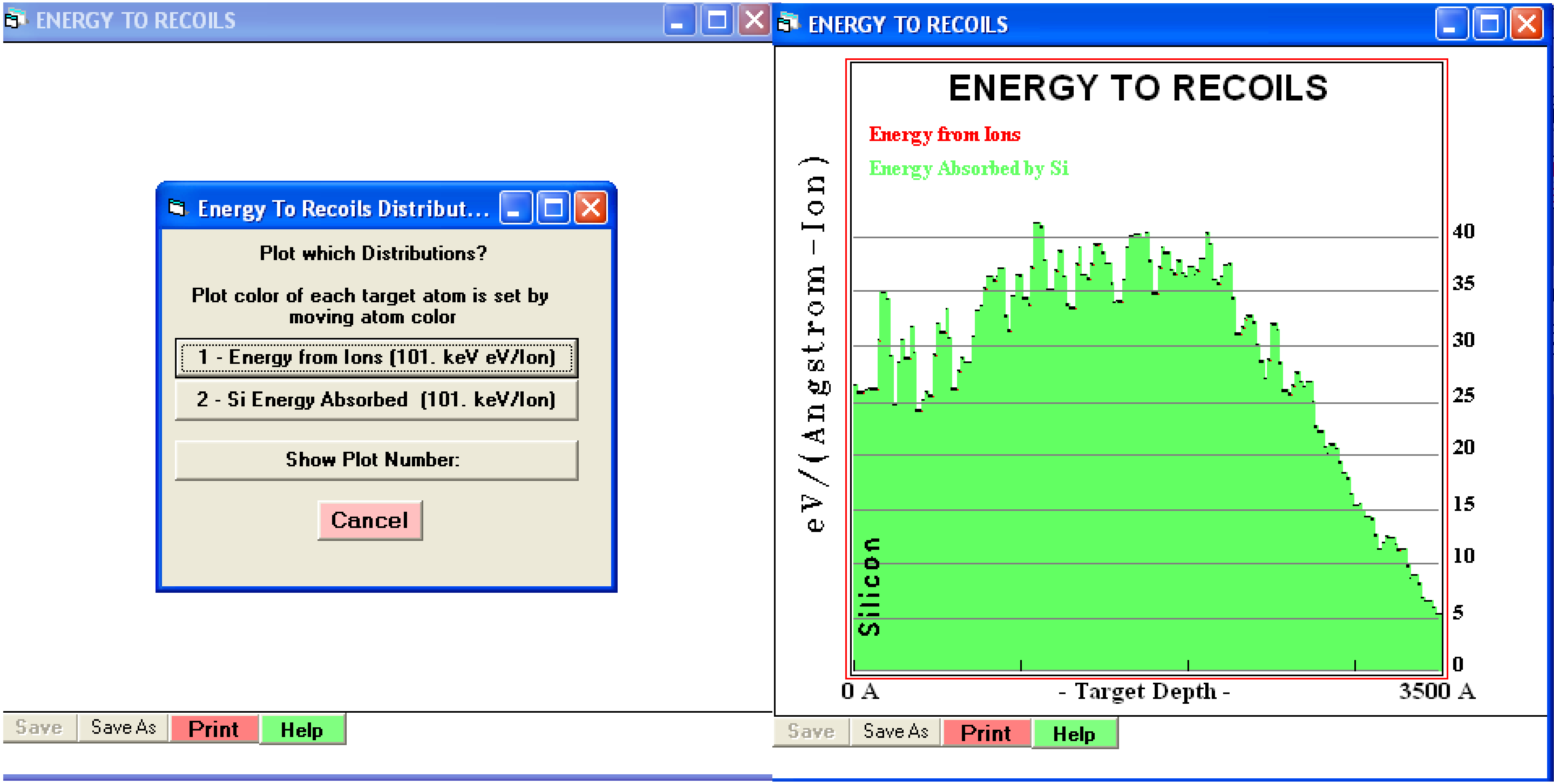
Recoils: 190 keV x 29% = 55 keV





% ENERGY LOSS	Ions	Recoils
Ionization	45.22	23.24
Vacancies	0.13	2.47
Phonons	0.44	28.49

➢ Damage Creation in the Target



Plot which Distributions?

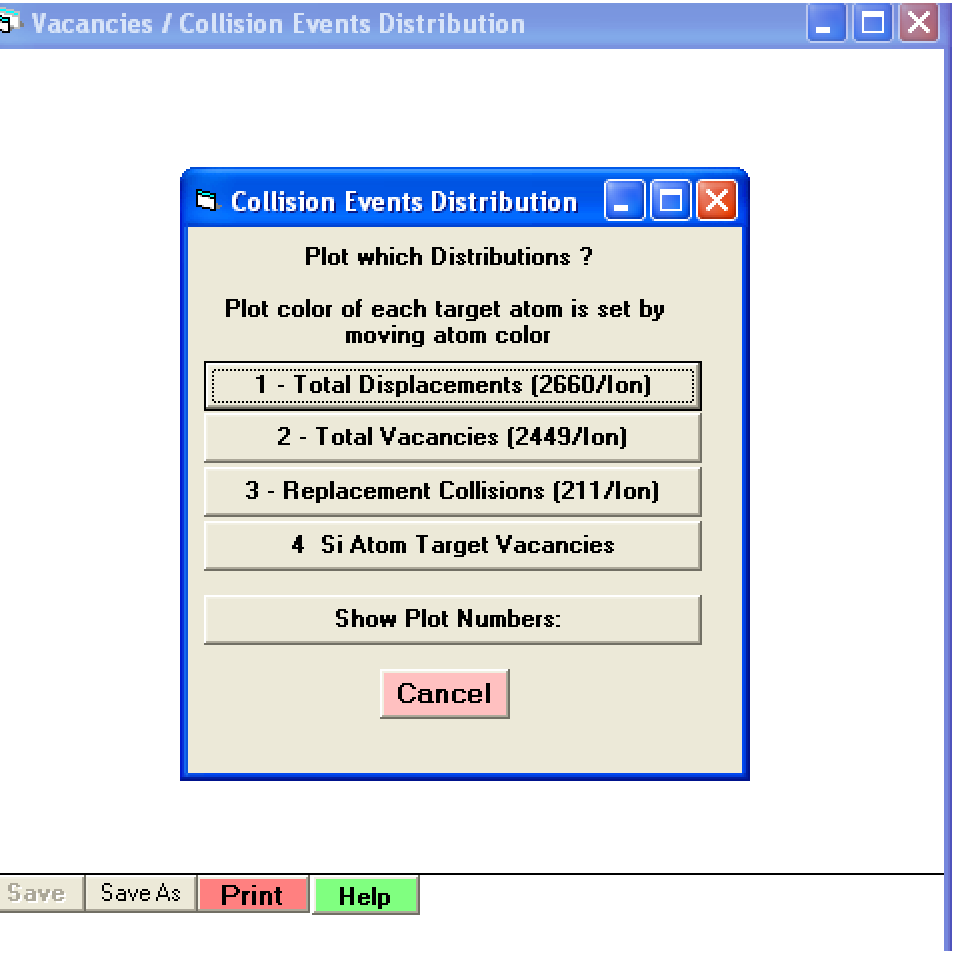
Plot color of each target atom is set by moving atom color

1 - Energy from Ions (101. keV eV/Ion)

2 - Si Energy Absorbed (101. keV/Ion)

Both plots are identical for a single element target, since all the energy deposited by the ions will be absorbed by silicon atoms.

➢ Damage Creation in the Target



Plot which Distributions ?

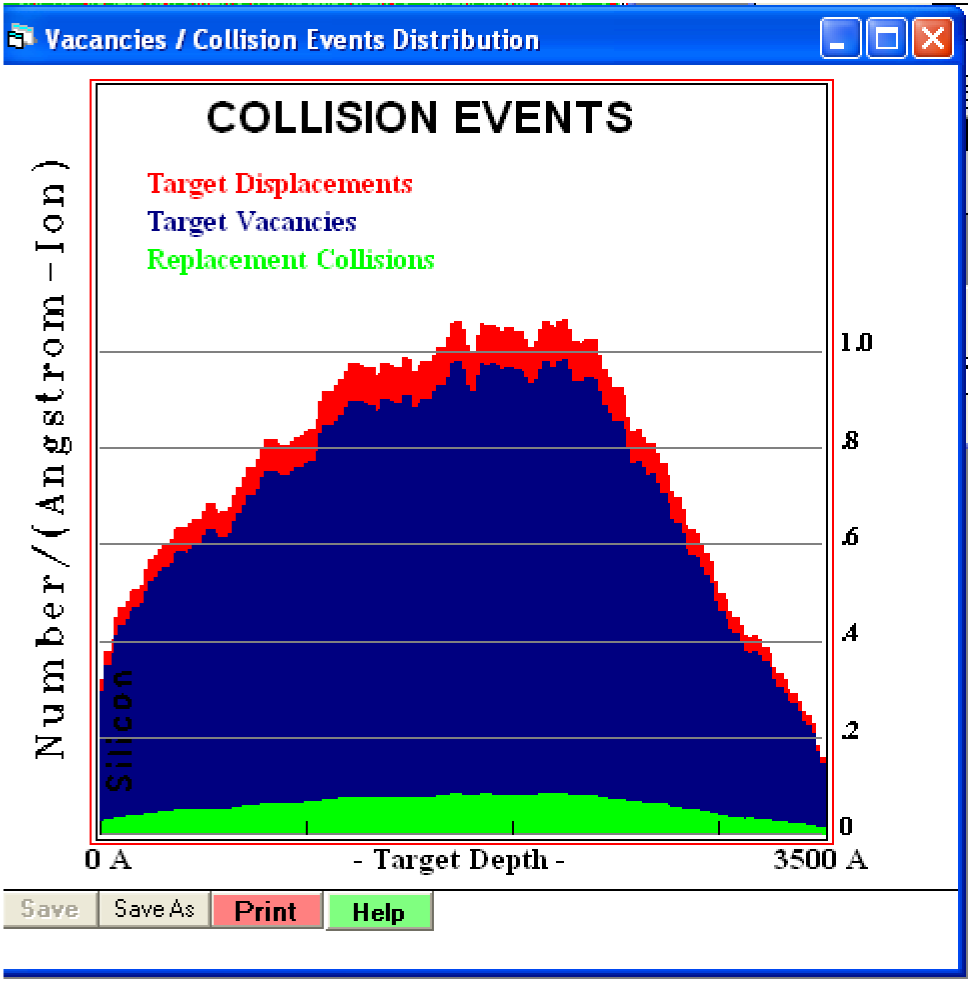
Plot color of each target atom is set by moving atom color

1 - Total Displacements (2660/Ion)

2 - Total Vacancies (2449/Ion)

3 - Replacement Collisions (211/Ion)

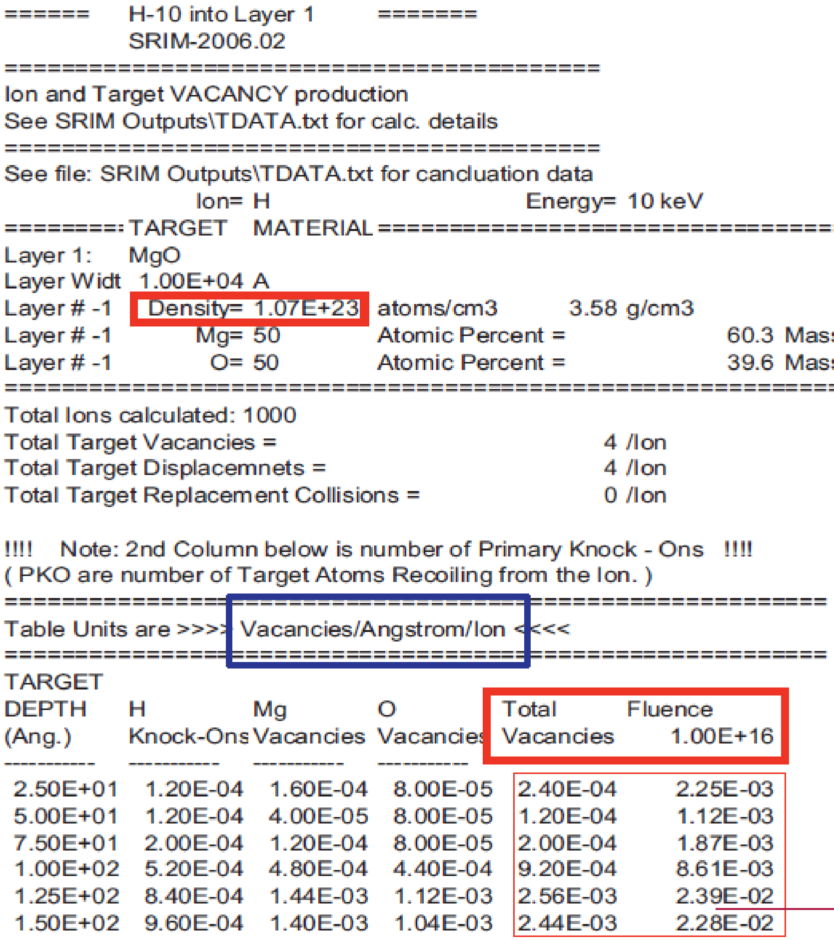
4 Si Atom Target Vacancies



Total Displacements = Total Vacancies + Replacement Collisions

DPA Calculation

VACANCY File



```
======     H-10 into Layer 1        =======
           SRIM-2006.02
=============================================
Ion and Target VACANCY production
See SRIM Outputs\TDATA.txt for calc. details
=============================================
See file: SRIM Outputs\TDATA.txt for cancluation data
                Ion= H                          Energy= 10 keV
=========: TARGET   MATERIAL ======================================
Layer 1:   MgO
Layer Widt  1.00E+04 A
Layer # -1   Density= 1.07E+23  atoms/cm3        3.58 g/cm3
Layer # -1          Mg= 50      Atomic Percent =             60.3 Mass Percent
Layer # -1           O= 50      Atomic Percent =             39.6 Mass Percent
=========================================================================
Total Ions calculated: 1000
Total Target Vacancies =                         4 /Ion
Total Target Displacemnets =                     4 /Ion
Total Target Replacement Collisions =            0 /Ion

!!!!   Note: 2nd Column below is number of Primary Knock - Ons   !!!!
( PKO are number of Target Atoms Recoiling from the Ion. )
==============================================================
Table Units are >>>> Vacancies/Angstrom/Ion <<<<
==============================================================
TARGET
DEPTH      H          Mg         O          Total       Fluence
(Ang.)     Knock-Ons  Vacancies  Vacancies  Vacancies    1.00E+16
---------- ---------- ---------- ----------
 2.50E+01   1.20E-04   1.60E-04   8.00E-05  2.40E-04     2.25E-03
 5.00E+01   1.20E-04   4.00E-05   8.00E-05  1.20E-04     1.12E-03
 7.50E+01   2.00E-04   1.20E-04   8.00E-05  2.00E-04     1.87E-03
 1.00E+02   5.20E-04   4.80E-04   4.40E-04  9.20E-04     8.61E-03
 1.25E+02   8.40E-04   1.44E-03   1.12E-03  2.56E-03     2.39E-02
 1.50E+02   9.60E-04   1.40E-03   1.04E-03  2.44E-03     2.28E-02
```

- Import vacancy file into EXCEL (deliminator is space)
- Add the total vacancies (all element types)
- Insert the calculated fluence (during experiments this is typically measured)

→ dpa

Courtesy of Prof. Gao at Umich

DPA Calculation

- Experiments

$$\text{Current} = I = \frac{C}{s} = \frac{\text{Ions} * q}{s}$$

A = area of the ion beam cross section

q = ion charge

ρ = sample density

M = mass number of sample

$$\text{Flux} = \phi = \frac{\text{ions}}{\text{cm}^2 - \text{s}} = \frac{I}{q * A}$$

$$\text{Fluence} = \text{Flux} * \text{time} = \phi * t = \Phi = \frac{\text{ions}}{\text{cm}^2}$$

$$\text{Number density} = N = \frac{\rho * N_A}{M}$$

- SRIM calculation

D = damage rate to sample from SRIM calculation (peak)

$$= \frac{\text{vacancies}}{\text{ion-Angstrom}}$$

$$\text{dpa}_{\text{rate}} = \frac{D * \phi}{N} = \frac{\text{vacancies}}{\text{ion} - \text{cm}} \frac{\text{ions}}{\text{cm}^2 - \text{s}} / \frac{N_a}{\text{cm}^3} = \frac{\text{vacancies}}{N_a \text{s}}$$

$$\text{dpa} = \frac{D * \Phi}{N} = \frac{\text{Total vacancies}}{N_a}$$

Watch Units!!

Courtesy of Prof. Gao at Umich

Thanks for your attentions!