Introduction of SRIM

Simulation Section of Nuclear Materials Experiment

Jingyi Shi

On behalf of prof. Lei Peng

School of Nuclear Science and Technology, University of Science and Technology of China, Hefei, Anhui 230026 China

2017-04-01

SRIM: The Stopping and Range of Ions in Matter
by James Ziegler

TRIM (the Transport of Ions in Matter)

SRIM or TRIM is a collection of software packages which calculate many features of the transport of ions in matter.

http://www.srim.org

- Background
- Installing of SRIM
- Introduction of SRIM
- SRIM Application

- **Background**
- Installing of SRIM
- Introduction of SRIM
- SRIM Application

名词解释

Ion :入射粒子　　Atom :靶原子

Recoil atoms: 与入射粒子发生位移碰撞的反冲靶原子

Cascade:由于一个初级撞出原子而导至众多的原子发生位移的过程

Vacancy: 晶格中某个原子被移去后所形成的缺陷

Interstitial atoms:填隙原子是指在正常排列的晶格原子位置之间插入的多余原子.

Backscattered Ions:从入射表面进来又从入射表面出去的入射粒子

Transmitted Ions:从入射表面进来从背面出去的入射粒子

Sputtered atoms:被入射粒子碰撞而离开入射表面的靶原子

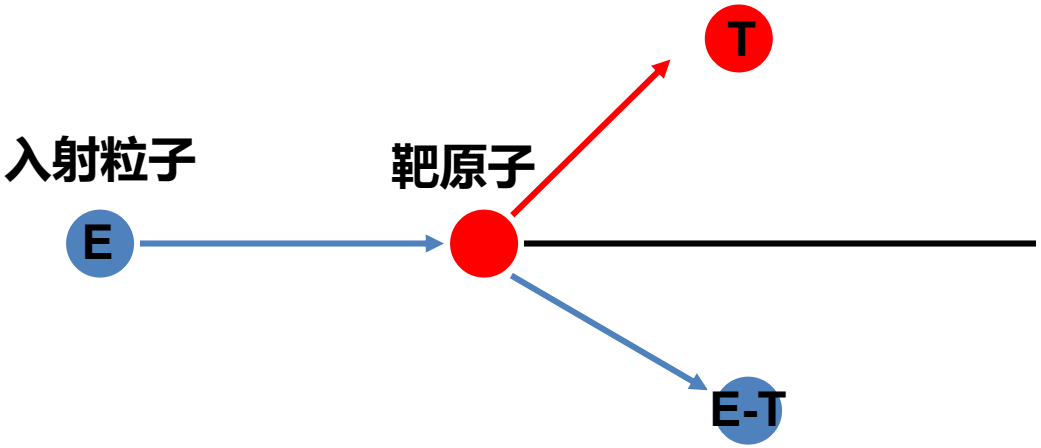
阻止本领（stopping power）

阻止本领（stopping power）： 入射粒子在物质中穿行将逐渐损失能量，能量损失过程的特征就用单位路径长度上的能量损失(-dE/dx)来描述。

单位路径长度上的核碰撞和电子碰撞能量损失分别称为核阻止本领(-dE/dx) nuclear和电子阻止本领(-dE/dx) elec。单位：eV/nm。

质量阻止本领： 表示带电粒子通过单位质量厚度物质时由于碰撞损失的能量。单位：keV/(mg.cm-2)

阻止本领（stopping power）



$$T_m = \Lambda E$$

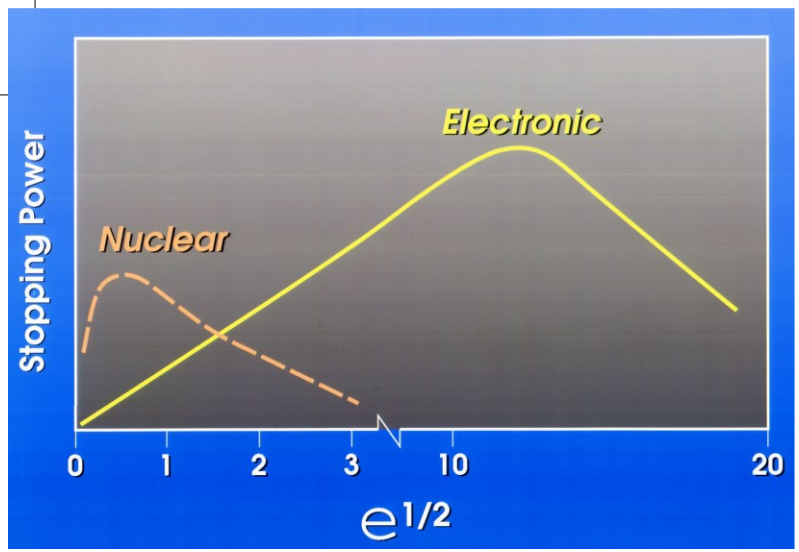
$$\Lambda = \frac{4M_1M_2}{(M_1+M_2)^2}$$

核阻止本领

$$\left.\frac{dE}{dx}\right|_N = \int_0^{\Lambda E} N\sigma(E,T)dT$$

电子阻止本领

$$\left(\frac{dE}{dx}\right)_e = k\sqrt{E}$$



Courtesy of Prof. Wang at Umich

射程（Range）

Range： 入射粒子从进入靶起到停止点所通过的总的路程, 称为射程.

Projected Range: 以Rp表示射程在入射方向投影的长度, 称作投影射程.

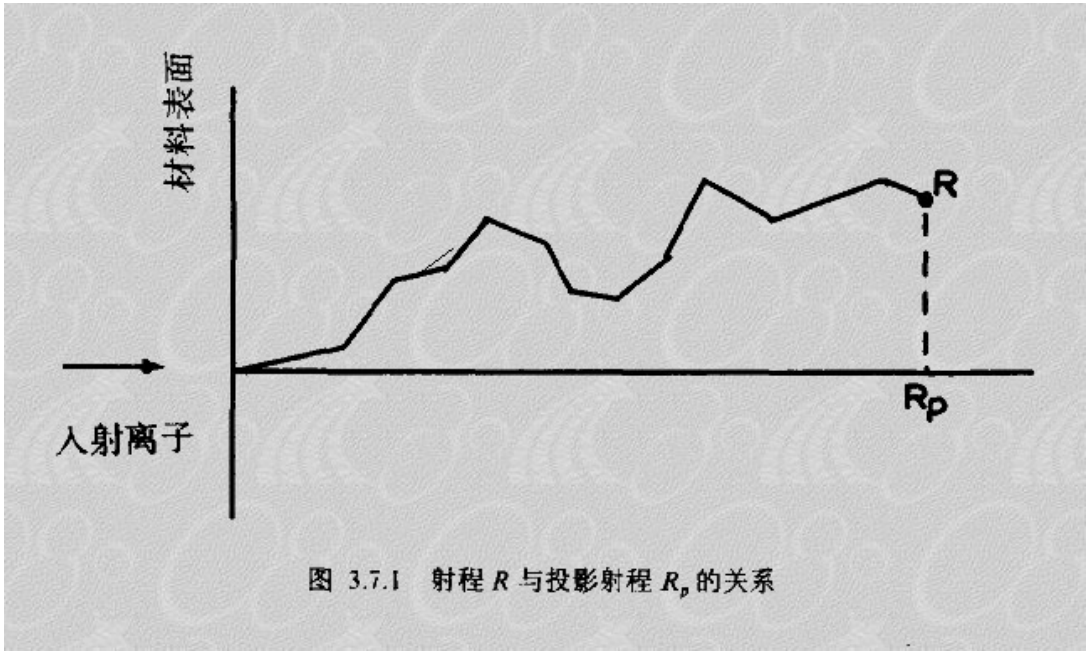


图 3.7.1 射程 R 与投影射程 R_p 的关系

射程（Range）

Mean Projected Range
平均投影射程：

$$R_p = \frac{\sum_i x_i}{N}$$

x_i 表示第i个入射粒子在X方向的投影射程

Lateral Projected Range:

$$R_y = \frac{\sum_i |y_i|}{N}$$

Radial Range:

$$R_r = \frac{\sum_i \sqrt{y_i^2 + z_i^2}}{N}$$

Straggle:

射程是具有统计性质的,不完全一致,而有小的统计变化

$$\sigma = \sqrt{\frac{\sum_i x_i^2}{N} - R_p^2}$$

入射过程中的碰撞

- 入射粒子先与靶原子的电子碰撞，称为原子碰撞（或电子碰撞），原子碰撞的结果是将靶原子的电子激发到高能量状态，即电离效应。
- 入射粒子在穿越电子云后与靶的原子核发生碰撞，称为原子核碰撞，通常的结果是将靶原子弹出晶格位置。即离位效应。

✓ *Displacement Collisions : The process where an energetic incident atom knocks a lattice atom off its site.*

✓ *Replacement Collisions : Atom sites with new atoms, identical to their original atom . This is the only mechanism in which a vacancy may be re-occupied.*

碰撞过程时的能量传递

入射粒子的能量损失过程分为两种：

- ✓ 一种是与靶原子核之间通过库仑作用发生的弹性碰撞而引起的，称为原子核能量损失过程。
- ✓ 另一种是激发电子，使其发生电离，即所谓的非弹性碰撞。称为电子能量损失。

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.

四种与碰撞有关的能量

✓*Displacement Energy*（离位阈能）:发生原子位移所必须的最小能量。

✓*Lattice Binding Energy*: 反冲靶原子离开晶格点阵时损失的能量

✓*Surface Binding Energy*：靶原子离开材料表面所需要克服的能量。用于计算溅射产额。

✓*Final Energy*(of a moving atom):below which it is considered to be stopped .

Displacement Energy

Displacement threshold energies

- For metals: 20-40 eV
- It is orientation dependent

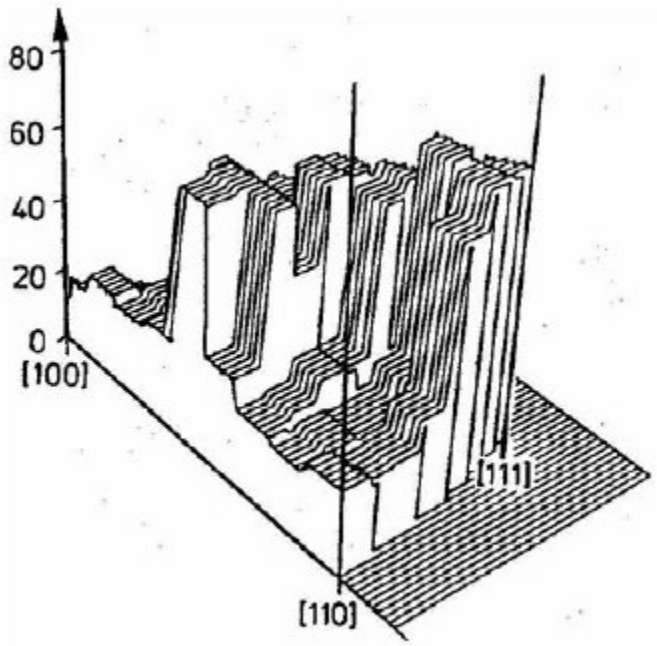


Table 7.1. *The minimum and average displacement threshold energies for some monatomic materials*

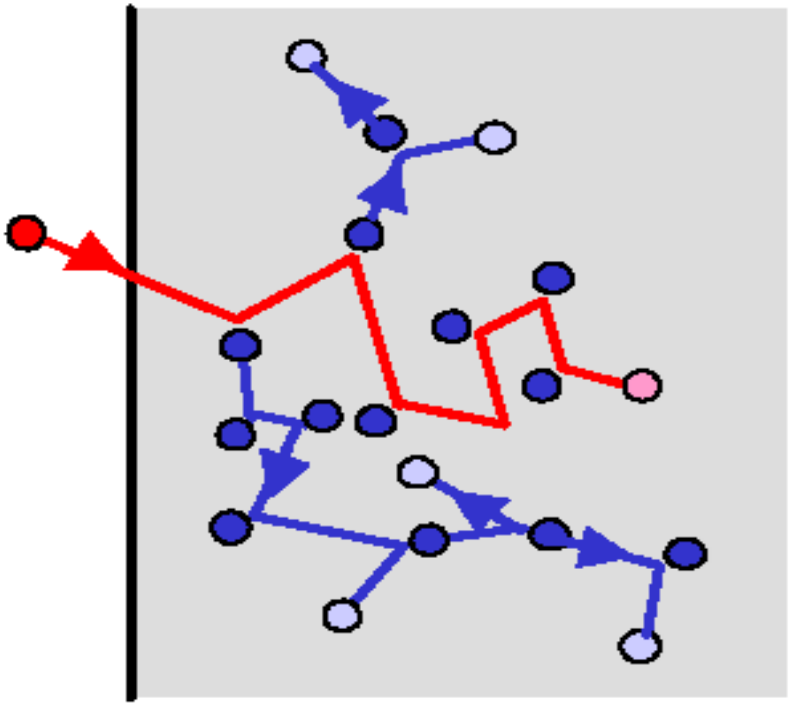
Atomic number	Chemical symbol	Minimum displacement energy (eV)	Average displacement energy (eV)
6	graphite	25	
6	diamond	35	
12	Mg	10	(20)
13	Al	16	27
14	Si	13	
22	Ti	19	(30)
23	V	26	
24	Cr	28	(60)
26	Fe (bcc)	17	(44)
27	Co (hcp)	22	34
28	Ni	23	34
29	Cu	19	29
30	Zn	14	29
31	Ga	12	
32	Ge	15	
40	Zr	21	(40)
41	Nb	28	(78)
42	Mo	33	(65)
46	Pd	26	41
47	Ag	25	39
48	Cd	19	36
49	In	15	
50	Sn (white)	22	
50	Sn (gray)	22	
71	Lu	17	
73	Ta	34	90
74	W	38	(110)
75	Re	40	(60)
78	Pt	33	44
79	Au	36	43
82	Pb	14	19
90	Th	35	44

Threshold values compiled from H. H. Andersen, *Appl. Phys.* **18** (1979), 131; and P. Lucasson, in *Fundamental Aspects of Radiation Damage in Metals*, M. T. Robinson and F. W. Young, Jr, eds. (US GPO, Washington, D.C., 1976), vol. 1, p. 42.

Courtesy of Prof. Wang at Umich

Cascade 级联过程

❖ PKA：靶原子获得的能量大于移位阈能时（ > Ed ），将离开它的晶格位置。第一个被入射粒子撞出的靶原子。



• **级联碰撞（ collision cascade ）**

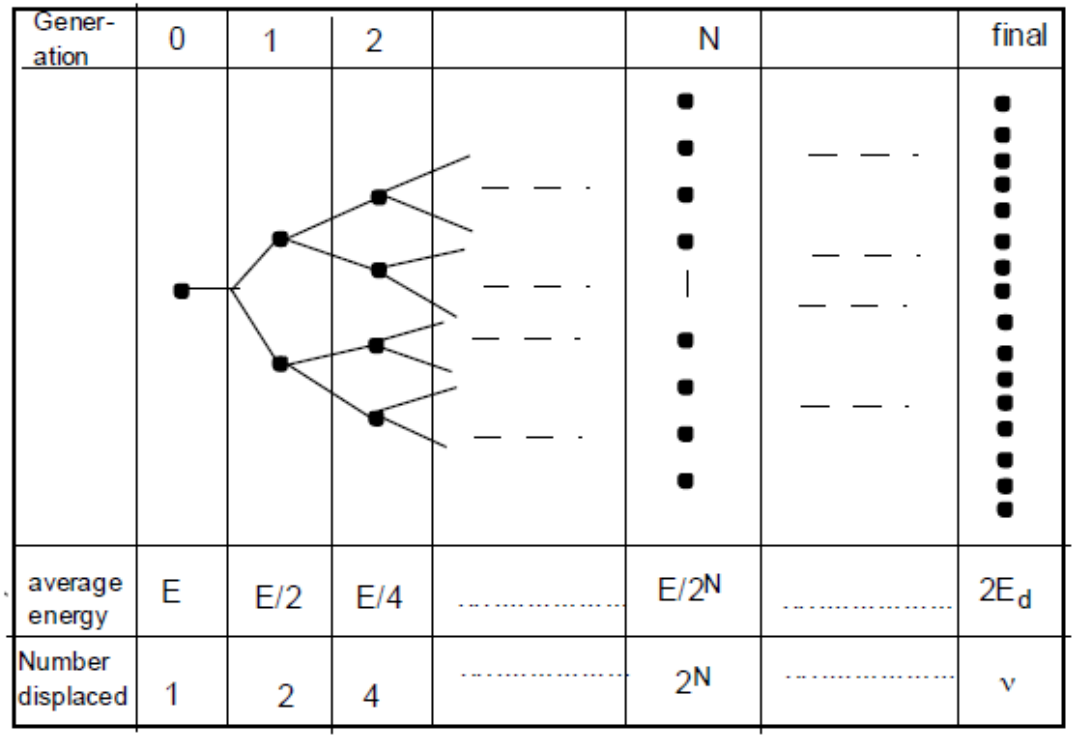
PKA 能量如果与离位阈能相比足够大，可以像入射粒子一样，将晶格原子从晶格位置上撞击出来。

入射粒子产生级联碰撞的示意图

Kinchin-Pease Model

Lattice Displacements Due to a Single PKA

- $E \leq E_d$ - no displacements
- $E_d \leq E \leq 2E_d$ - only PKA displaced ($T < E_d$)
- For $E > 2E_d$



(Kinchin-Pease model)

Cascade ceases when average knock-on energy is $2E_d = \frac{E}{2^{N_f}}$

Kinchin-Pease Model

The Kinchin-Pease Model

- Cascade ceases when average knock-on energy is

$$2E_d = \frac{E}{2^{N_f}}$$

- Final number of displaced atoms = $\nu = 2^{N_f}$

$$\nu = \frac{E}{2E_d}$$

Courtesy of Prof. Wang at Umich

Kinchin-Pease Model

Summary on Displacement per PKA

The Kinchin-Pease model:

$$\nu_{KP}(E) = \frac{E}{2E_d}$$

$$\nu(E) = \frac{E^*}{2E_d} \quad if\ E > E^*$$

$$\nu(E) = \frac{E}{2E_d} \quad if\ 2E_d < E < E^*$$

$$\nu(E) = 1 \quad if\ E_d < E < 2E_d$$

$$\nu(E) = 0 \quad if\ E < E_d$$

$E^* = M_1$ (keV)
minimum ion energy for transferring enough energy to an electron to remove it from the atom

E_d = displacement energy

$$\langle N_d(E) \rangle = \frac{E}{2E_d} \quad (\text{for } 2E_d < E < E_c) \qquad (7.13)$$

Courtesy of Prof. Wang at Umich

Kinchin-Pease Model

The total Kinchin–Pease PKA damage function can now be constructed from the combination of Eqs. (7.3), (7.13), and (7.14)

$$\langle N_d(E)\rangle = \begin{cases} 0 & (\text{if } E < E_d) \\ 1 & (\text{if } E_d < E < 2E_d) \\ E/2E_d & (\text{if } 2E_d < E < E_c) \\ E_c/2E_d & (\text{if } E > E_c) \end{cases} \tag{7.15}$$

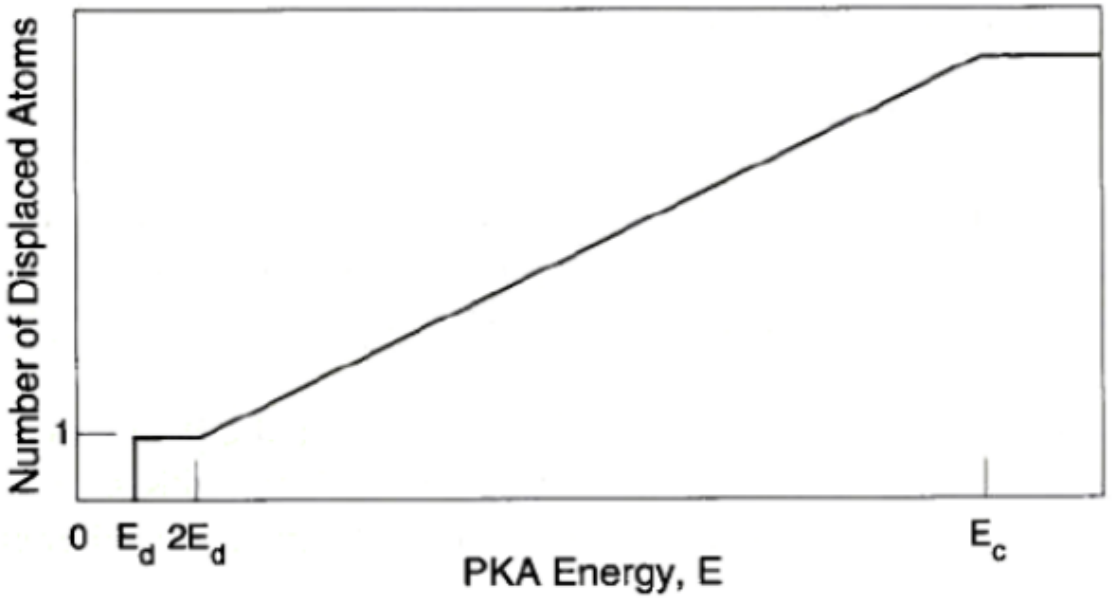
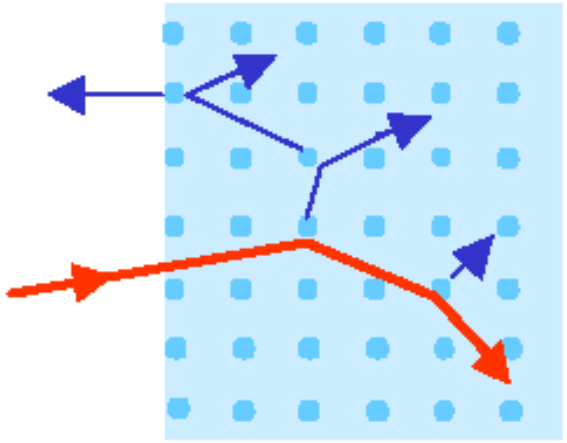


Fig. 7.6. A graphical representation of the number of displaced atoms in the cascade as a function of PKA energy according to the model of Kinchin and Pease, Eq. (7.15).

Courtesy of Prof. Gao at Umich

表面溅射Sputtered ions

- ✓ 一定能量的离子打到固体表面时，会使表面部分原子、分子或原子团出射，这一现象叫做表面溅射。
- ✓ 溅射机理，当碰撞级联延伸到表面，使表面的原子能量足以克服表面结合能时，表面的原子便逸出成为溅射粒子。
- ✓ 溅射产额，定义为移出固体表面的原子数与入射粒子数之比，
- ✓ 溅射阈能，入射粒子能量大于此阈值时，才能发生溅射现象。此能量阈值的大小和靶材料以及入射粒子种类有关



溅射示意图

- Background
- **Installing of SRIM**
- Introduction of SRIM
- SRIM Application

The way to download SRIM

- **WIFI connection : ustcnet**

- **The SRIM program can be downloaded from both of below websites.**

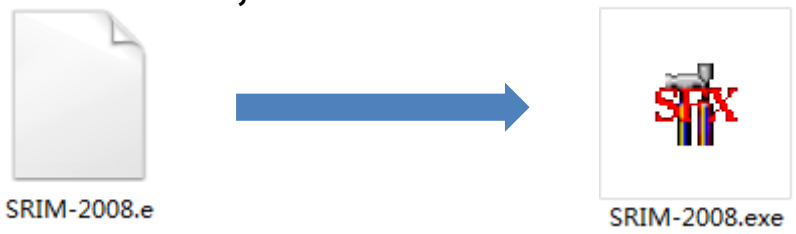
1. **Official website of SRIM： www.srim.org**
2. **My personal homepage: home.ustc.edu.cn/~shijy**

- **Three different version are available now.**

1. **SRIM-2008 (used in our course)**
2. **SRIM-2013_Standard (including Chinese tutorials and MS-linedraw font)**
3. **SRIM-2013_Professional (including 500 plots of (Experiment/Theory) stopping power, Chinese tutorials and MS-linedraw font)**

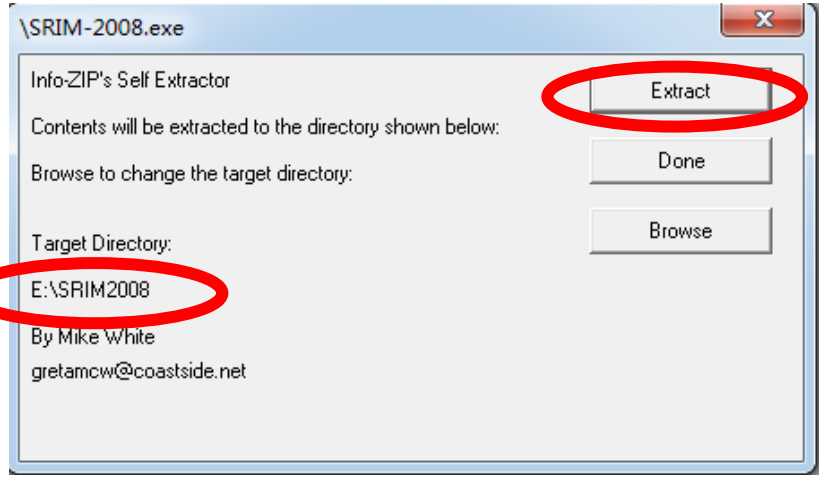
How to install SRIM? (use SRIM-2008 as example)

- **Put the installing package into a new directory (without Chinese path) called SRIM-2008, and rename the file to SRIM-2008.exe.**



- **Execute this renamed file to extract all the SRIM files.**

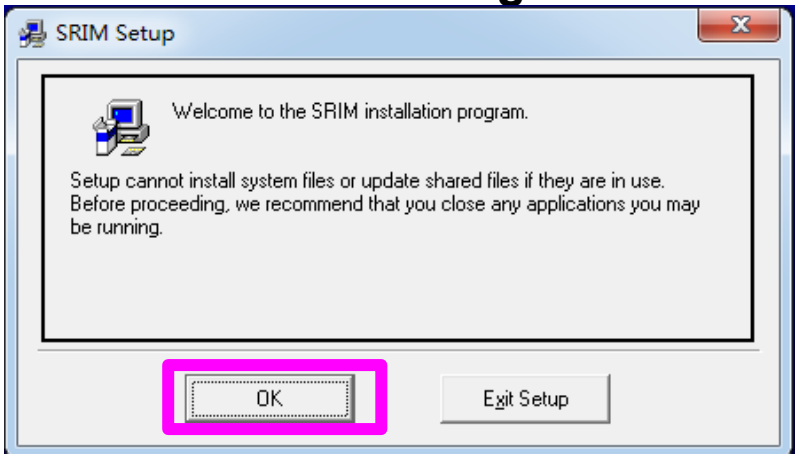
Non-Chinese directory path

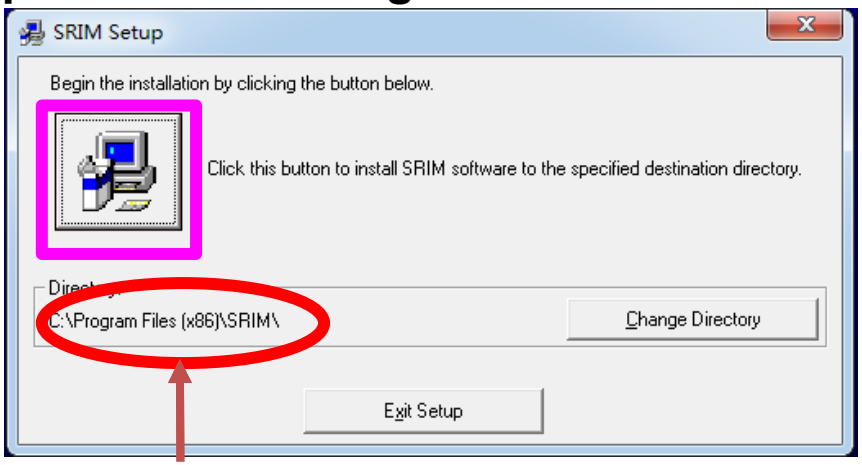


- **Double-click the SETUP.EXE file to trigger installing wizard.**

RICHED32.dl_	8/18/2001 10:00...	DL_ 文件	2 KB
RICHTX32.OC_	3/10/2004 6:45 ...	OC_ 文件	118 KB
S.bm_	6/24/1998 3:48 ...	BM_ 文件	1 KB
SCOEF03.da_	12/21/2002 11:5...	DA_ 文件	62 KB
SETUP.EXE	1/16/1997 1:00 ...	应用程序	88 KB
SETUP.LST	10/22/2008 6:27...	LST 文件	24 KB
setup1.ex_	1/16/1997 1:00 ...	EX_ 文件	72 KB
SNUC03.da_	9/13/2002 4:55 ...	DA_ 文件	120 KB

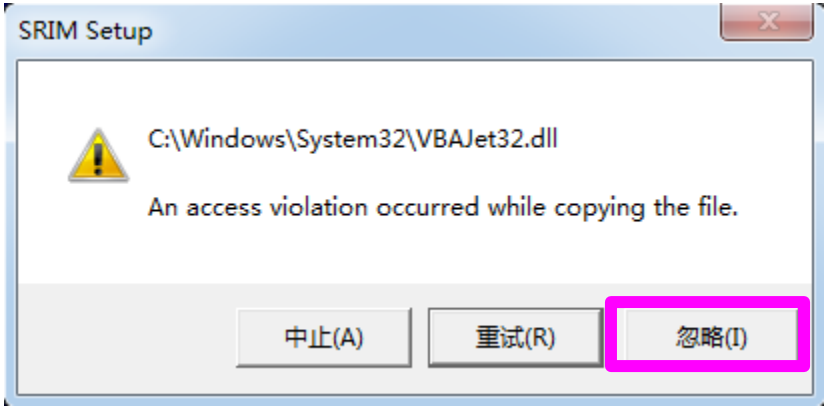
- **Click "OK" button, then choose the installing directory and click the installing button at the top left of the dialog box.**

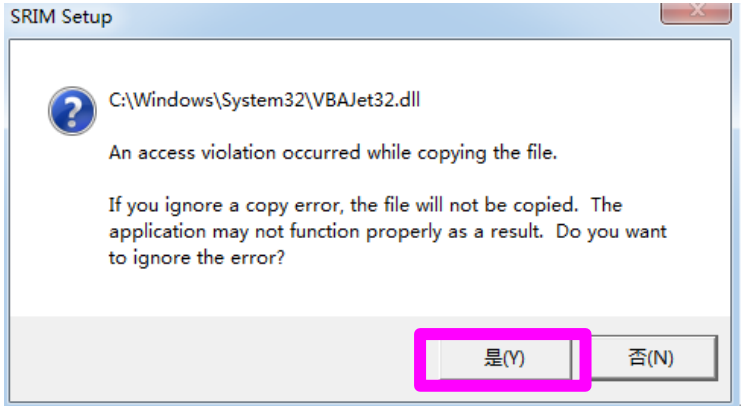


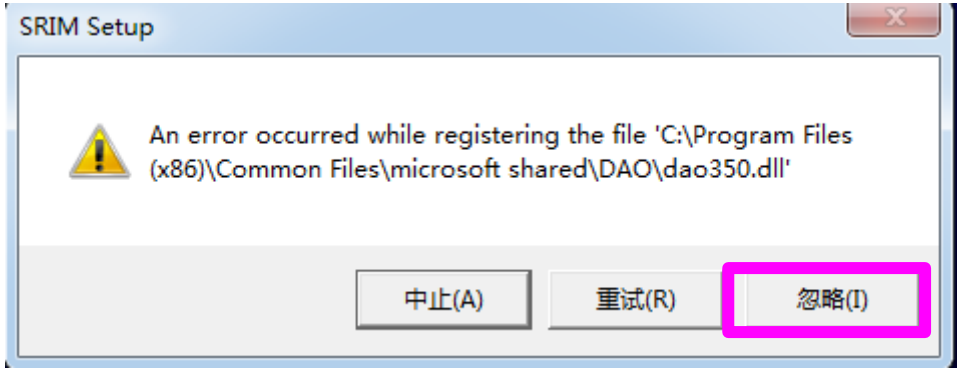


Non-Chinese directory path

- **Neglect the errors reminder during process of installing.**



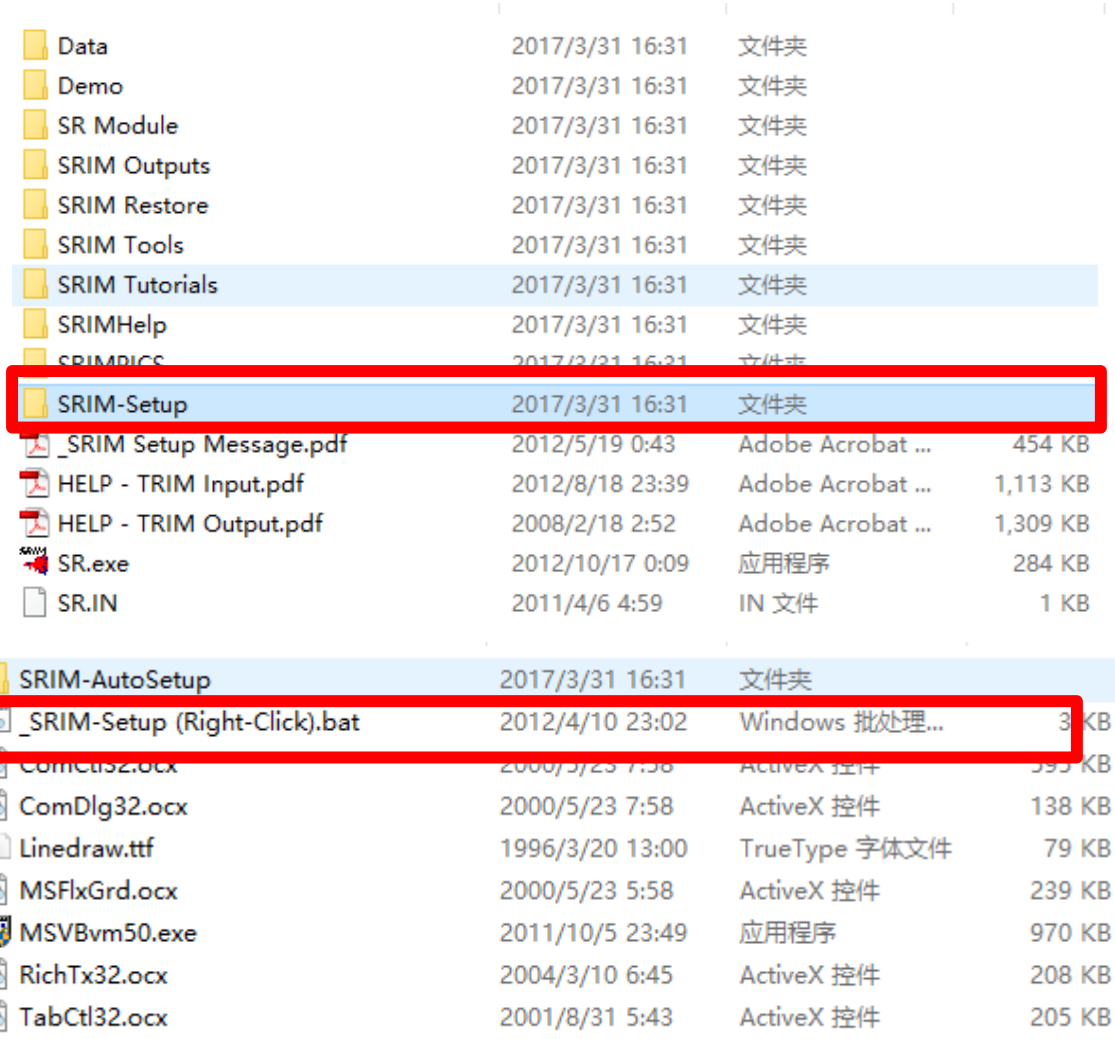




➢ Run SRIM

Name	Size	Type	Date Modified
Data		File Folder	3/31/2017 1:47 AM
Demo		File Folder	1/10/2017 6:24 AM
SR Module		File Folder	1/10/2017 6:25 AM
SRIM Outputs		File Folder	3/23/2017 2:15 AM
SRIM Restore		File Folder	3/31/2017 1:47 AM
SRIM Tools		File Folder	1/10/2017 6:25 AM
SRIM Tutorials		File Folder	1/10/2017 6:25 AM
SRIMHelp		File Folder	1/10/2017 6:25 AM
SRIMPICS		File Folder	1/10/2017 6:25 AM
HELP - TRIM Output.pdf	1,309 KB	PDF File	2/17/2008 11:52 AM
HELP - TRIM Setup and Input....	476 KB	PDF File	1/27/2008 7:30 AM
SR	282 KB	Application	7/23/2008 6:38 PM
SRIM 2008	706 KB	Application	7/23/2008 6:18 PM
SRIM LiesMich (German)	9 KB	Text Document	3/24/2003 5:24 PM
SRIM ReadMe	7 KB	Text Document	8/19/2007 7:44 PM
SRIM ReadMe (Chinese)	101 KB	Rich Text Document	11/13/2006 5:38 PM
SRIM ReadMe (English)	8 KB	Rich Text Document	8/19/2007 7:38 PM
SRIM ReadMe (French)	9 KB	Text Document	12/21/2002 10:54 PM
SRIM ReadMe (Spanish)	8 KB	Text Document	12/21/2002 9:02 PM
ST5UNST	28 KB	Text Document	1/10/2017 6:25 AM
TIN	714 KB	Application	8/12/2008 6:51 PM
TRIM	912 KB	Application	8/12/2008 6:19 PM
TRIM.IN	2 KB	IN File	1/12/2017 12:12 AM
TRIMAUTO	1 KB	File	1/12/2017 12:12 AM
TRIMAUTO	2 KB	Text Document	9/16/2002 6:42 PM

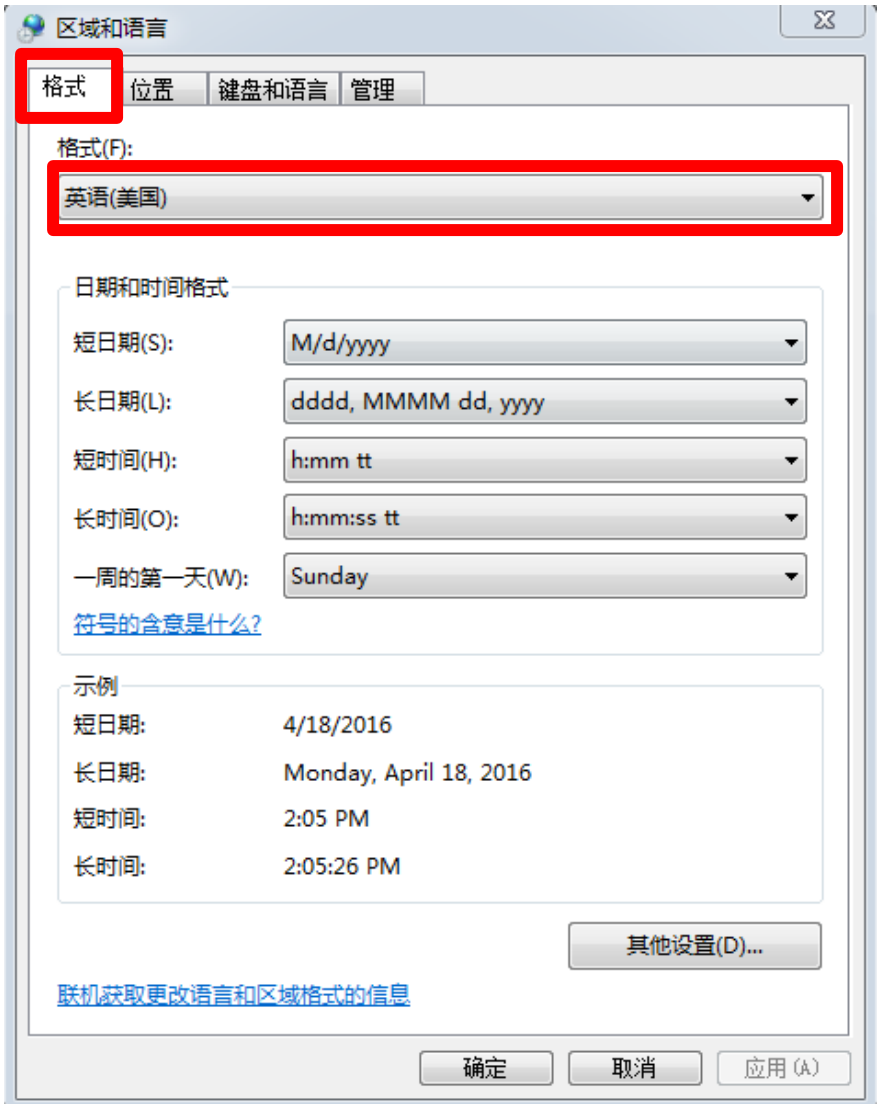
How to solve the problem of missing standard Windows files ?
(Specialize for SRIM-2013 installing in the Windows OS after XP)

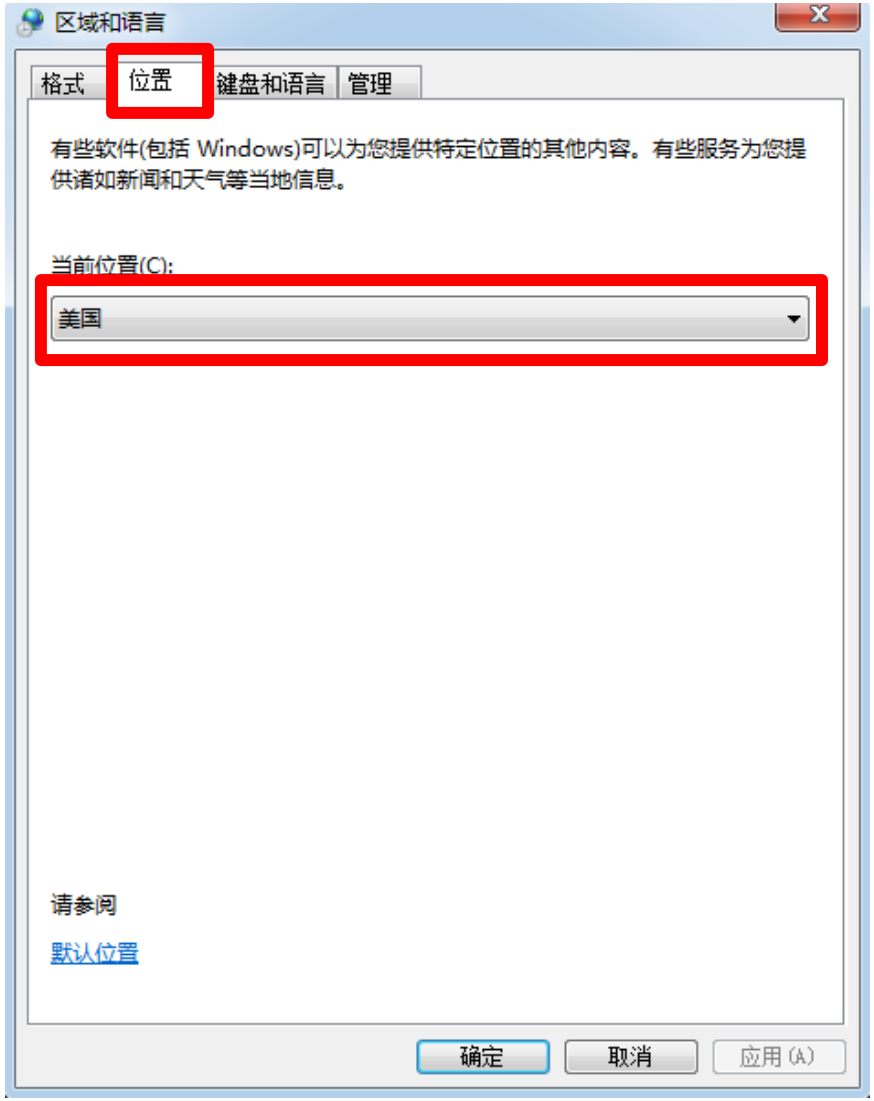


Right-Click and run as administration

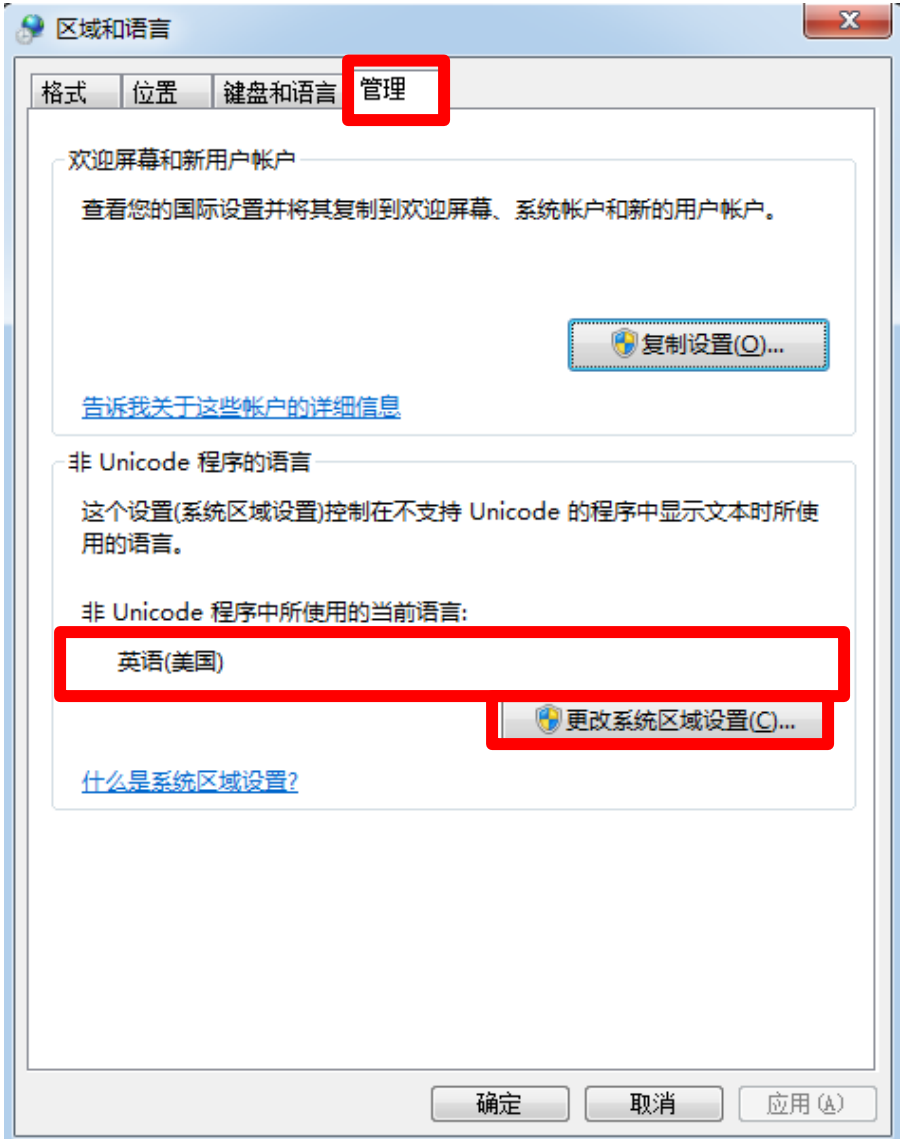
➢ How to solve TRIM Hangs-up?

➢ How to solve TRIM Hangs-up?





➢ How to solve TRIM Hangs-up?



Then reboot!

- Background
- Installing of SRIM
- **Introduction of SRIM**
- SRIM Application

SRIM:

The stopping and range of ions into matter.

入射粒子：ion　　靶原子： atoms

SRIM采用蒙特卡洛方法，通过计算机模拟跟踪一大批入射粒子的运动。粒子的位置、能量损失以及次级粒子的各种参数都在整个跟踪过程中存储下来,随机选定碰撞参数，模拟碰撞过程，计算入射离子从进入靶开始碰撞到最终丧失能量停止或穿出靶的过程。最后得到各种所需物理量的期望值和相应的统计误差。由于计算的结果具有统计意义，只有当计算的离子个数足够多，才能获得所需要的计算精度。

SRIM主要包括两个程序，SR和TRIM。

- **SR(Stopping and Ranges of ions in simple targets).** **quickly creates Tables of the stopping and range of ions in matter over a wide band of ion energies.**

- **TRIM (the Transport of Ions in Matter) is a Monte-Carlo calculation which follows the ion into the target, making detailed calculations of the energy transferred to every target atom collision. (multi-layer complex targets)**

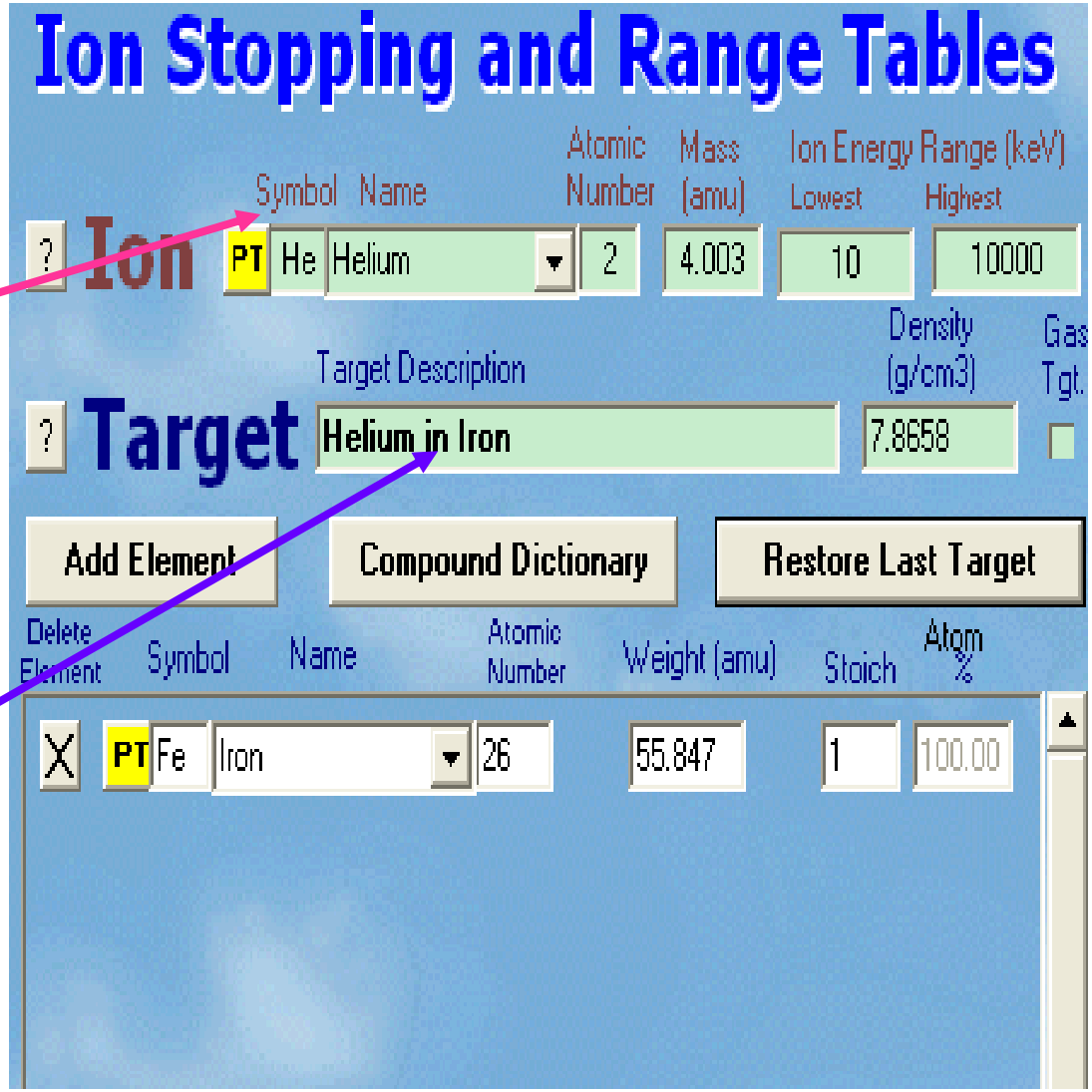
SR

入射粒子的数据

（元素，原子质量，入射粒子的数据入射粒子能量范围）

靶对象的数据

（元素，状态，原子质量，各成分所占比例）



我们可以得到：不同能量的入射粒子（10eV- 2×10^9 eV）在靶材料中的射程，原子核能量损失，电子能量损失，以及横向和纵向的stragge.

Disk File Name = SRIM Outputs\Helium in Iron

Ion = Helium [2] , Mass = 4.003 amu

Target Density = 7.8658E+00 g/cm3 = 8.4817E+22 atoms/cm3

======= Target Composition ========

Atom Name	Atom Numb	Atomic Percent	Mass Percent
Fe	26	100.00	100.00

==========

Bragg Correction = 0.00%

Stopping Units = MeV / (mg/cm2)

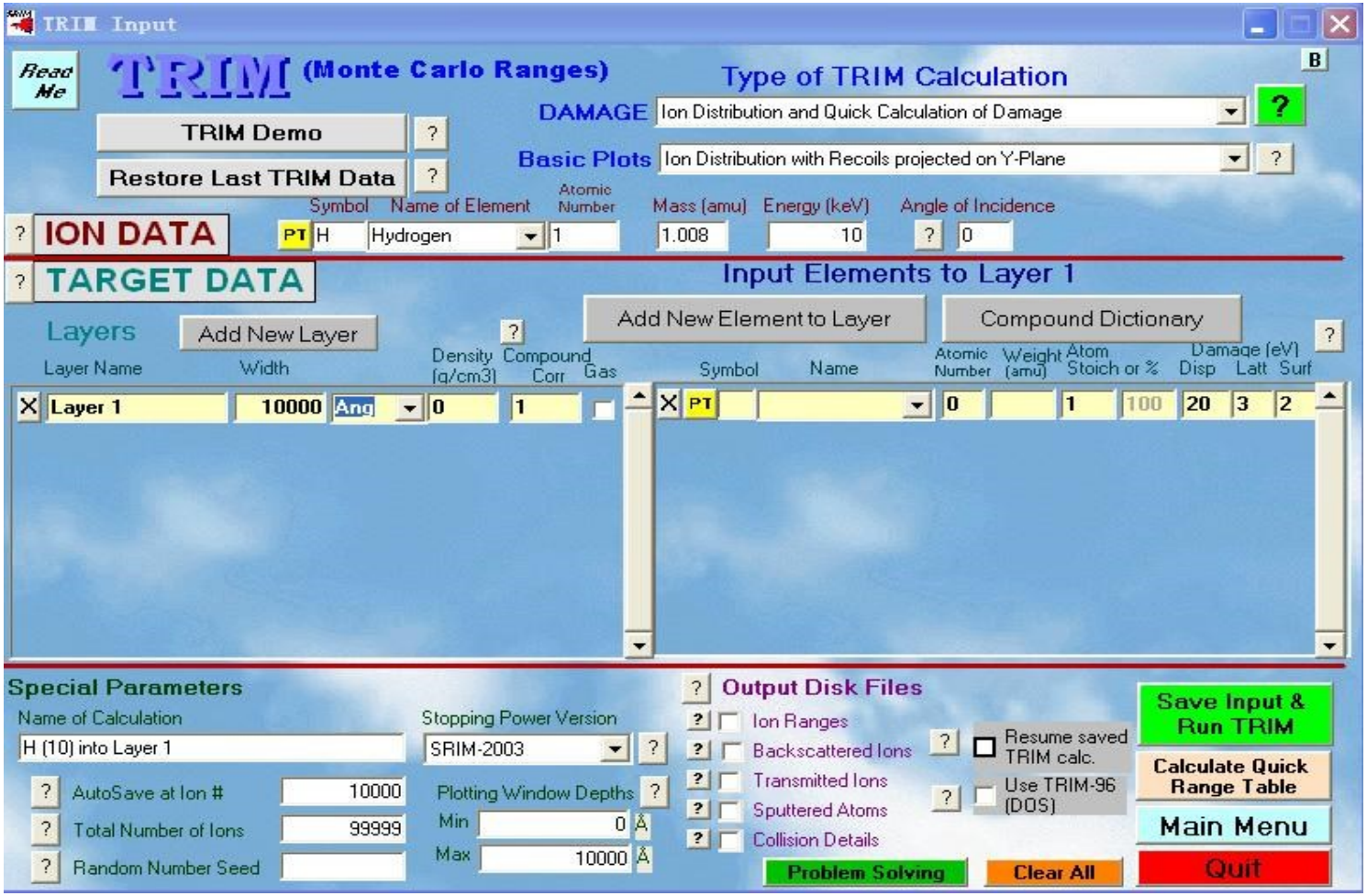
See bottom of Table for other Stopping units

Ion Energy	dE/dx Elec.	dE/dx Nuclear	Projected Range	Longitudinal Straggling	Lateral Straggling
10.00 keV	1.223E-01	2.606E-02	389 A	333 A	261 A
11.00 keV	1.261E-01	2.524E-02	429 A	356 A	281 A
12.00 keV	1.303E-01	2.448E-02	470 A	378 A	300 A
13.00 keV	1.359E-01	2.376E-02	510 A	399 A	319 A
14.00 keV	1.425E-01	2.310E-02	550 A	420 A	337 A
15.00 keV	1.496E-01	2.247E-02	590 A	439 A	354 A
16.00 keV	1.568E-01	2.189E-02	629 A	458 A	371 A
17.00 keV	1.639E-01	2.134E-02	667 A	475 A	387 A
18.00 keV	1.707E-01	2.082E-02	705 A	492 A	403 A

TRIM

可以设计成多层复合的靶（multi-layer complex targets），计算入射粒子入射后与靶原子各种相互作用以及能量转移，能够得到入射粒子在靶中的最终的**射程**、三维分布，以及得到靶的辐照损伤，表面的溅射，电离和声子的产生。

*TRIM*具体的输入表格和菜单



输入部分：

1) 入射粒子：

- ✓Name
- ✓Mass
- ✓Energy
- ✓Number 默认的是99999
- ✓Angle of Incidemce 默认的情况是粒子垂直靶表面入射。

2）靶：

✓width

✓*Elements*

✓Stoichiometry

靶材料的化学成分，比如SiO2,只要输入Si(1)O(2)就可以。

✓靶材料的密度（g/cm3）

对于单元素组成的层，TRIM程序自动给出元素的密度，但对于由混合物组成的层则要注意，TRIM程序根据元素各自的密度和化学组成算出来的密度值是否合理。

✓靶材料的总厚度

先用SR程序算出最大能量入射粒子的入射深度，有此确定靶材料的厚度，避免在模拟时，入射粒子的射程大于靶的厚度以致穿透靶材料。

3) Type of TRIM calculation

✓- Ion Distribution and Quick Calculation of Damage

建立在Kinchin-pease模型上，不关注靶损伤的详细情况或者溅射。快速计算一定能量粒子打进靶材料中的深度,可以计算

a:入射粒子在靶中的最终分布

b:电离能量损失

c:反冲靶原子，背散射入射粒子，透射粒子的能量转移

✓- Detailed Calculation with full Damage Cascades

该项跟踪每一个反冲核直到它们的能量低于靶原子的位移阈能.所有的级联碰撞损伤被考虑。计算入射粒子与靶原子的详细碰撞对靶物质的所有损伤。比如：溅射产额，入射粒子和反冲原子的能量损失详细情况。

✓- Calculation of Surface Sputtering

✓- Various Ion Energy / Angle / Positions

✓- Neutron / Electron / Photon Cascades

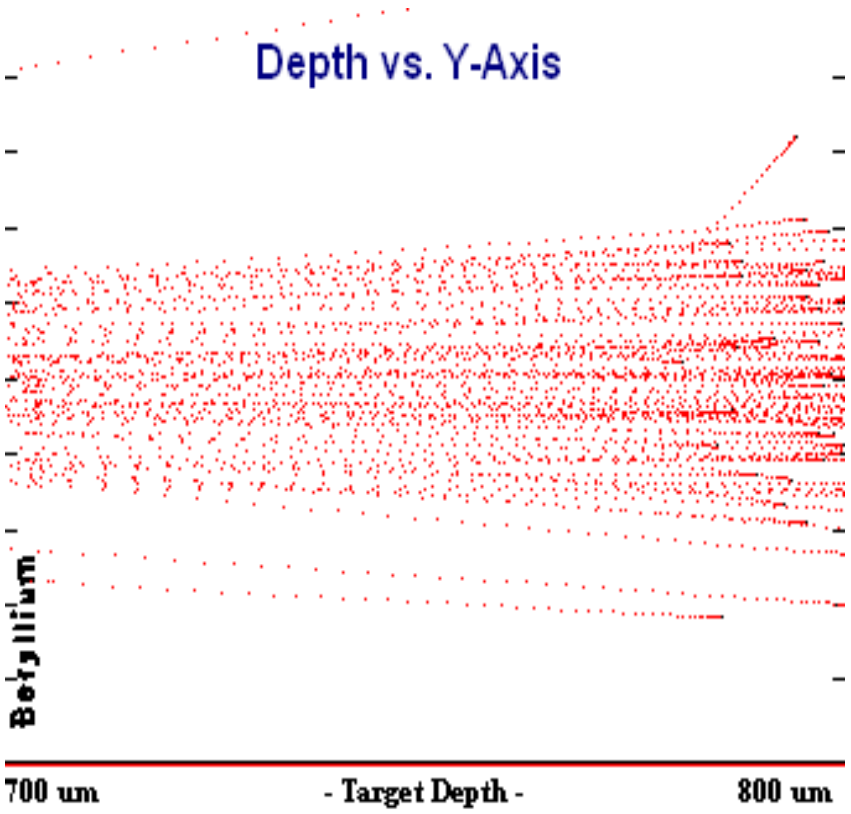
主要是计算靶原子受到中子，电子，光子碰撞后获得的能量以及级联过程在靶材料中引起的损伤。

4) calculation plots

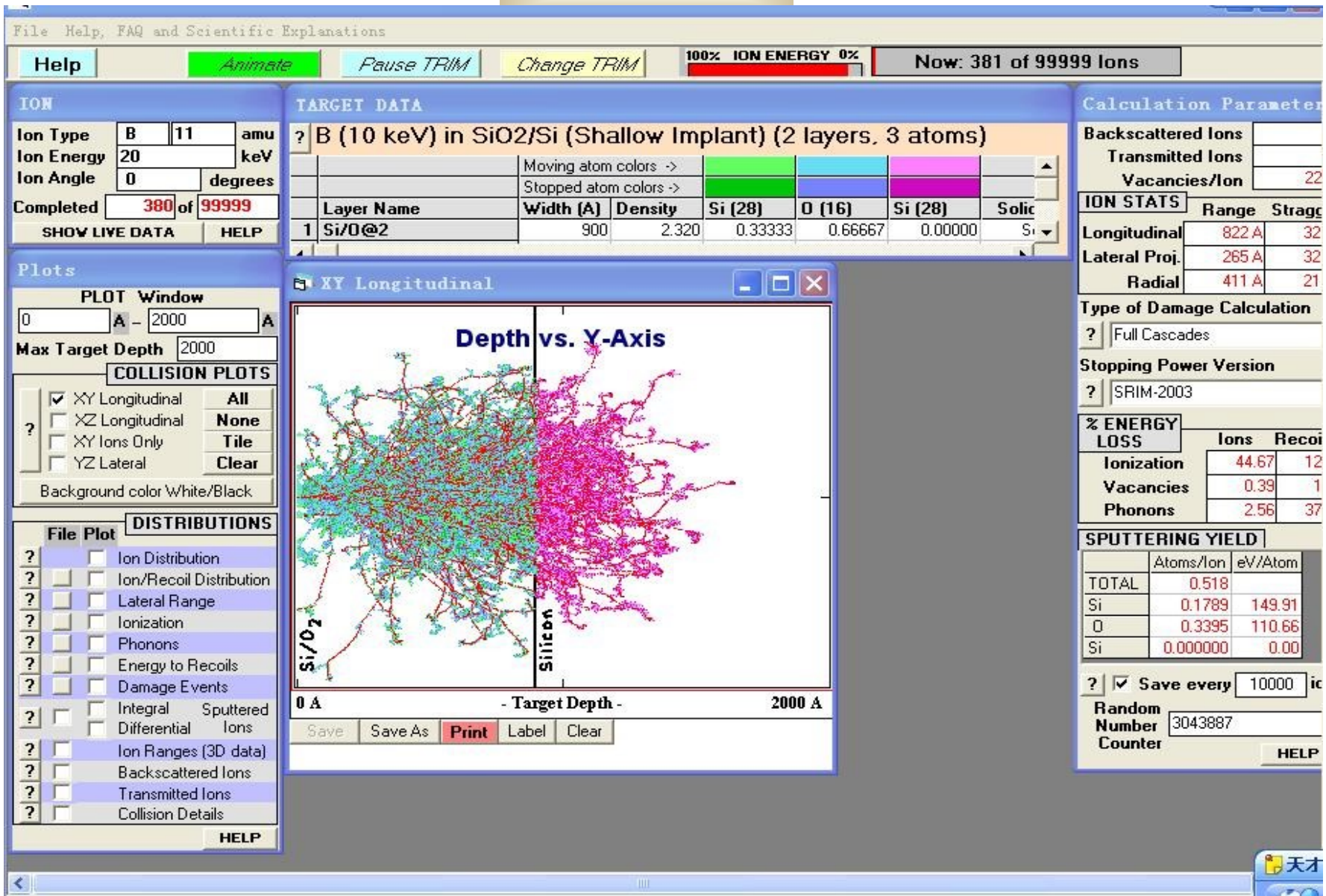
- ✓ Plot options:(定义垂直靶材料的方向为X方向)
  - ➢ Projection onto the XY plane.
  - ➢ Projection onto the XZ plane.
  - ➢ Ions only onto the XY plane.
  - ➢ Projection onto the YZ plane.

✓Plotting window depths
最后显示碰撞结果的视窗（Plotting window）的起止范围

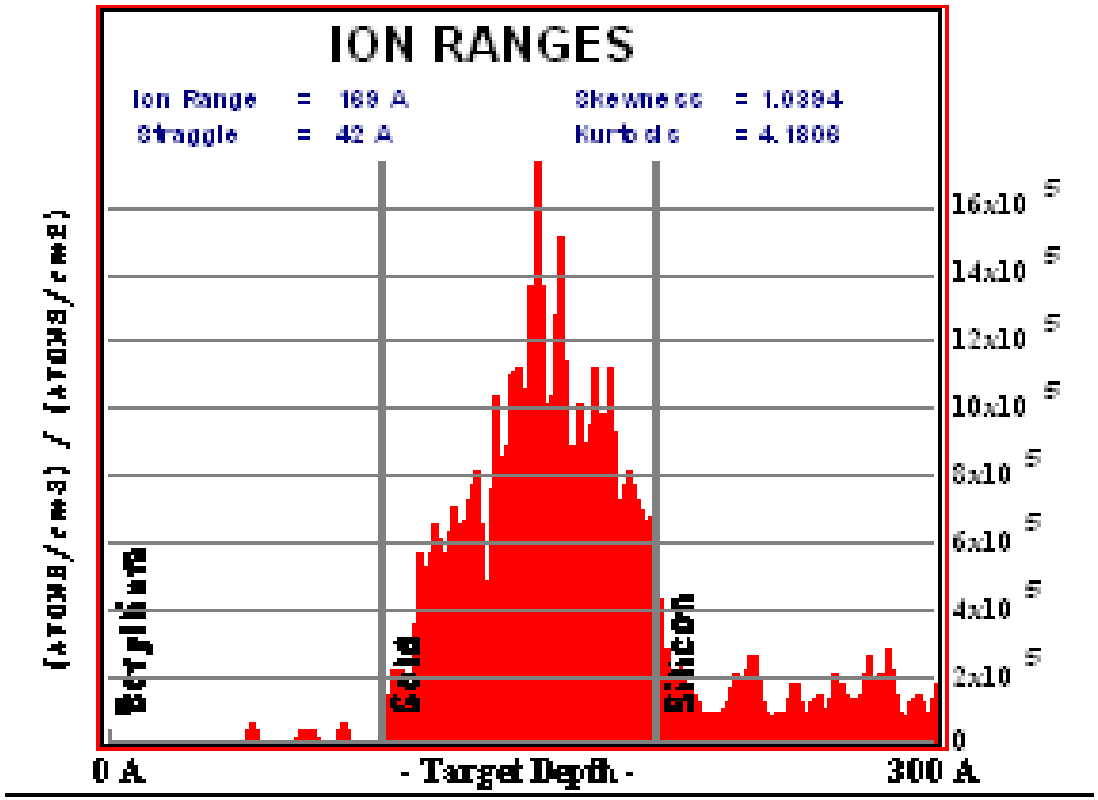
比如能量为10MeV的H入射Be靶中，射程是800μm，当设置的起止范围是700μm——800μm时，就能够观察到最后100μm的碰撞细节。



输出窗口


File Help, FAQ and Scientific Explanations
Help
Animate
Pause TRIM
Change TRIM
100% ION ENERGY 0%
Now: 381 of 99999 Ions
ION
Ion Type B 11 amu
Ion Energy 20 keV
Ion Angle 0 degrees
Completed 380 of 99999
SHOW LIVE DATA
HELP
TARGET DATA
B (10 keV) in SiO2/Si (Shallow Implant) (2 layers, 3 atoms)
Moving atom colors ->
Stopped atom colors ->
Layer Name
Width (A)
Density
Si (28)
O (16)
Si (28)
1 Si/O@2 900 2.320 0.33333 0.66667 0.00000
Calculation Parameter
Backscattered Ions
Transmitted Ions
Vacancies/Ion 22
ION STATS
Range
Longitudinal 822 A 32
Lateral Proj. 265 A 32
Radial 411 A 21
Type of Damage Calculation
Full Cascades
Stopping Power Version
SRIM-2003
% ENERGY LOSS
Ions
Recoi
Ionization 44.67 12
Vacancies 0.39 1
Phonons 2.56 37
SPUTTERING YIELD
Atoms/Ion
eV/Atom
TOTAL 0.518
Si 0.1789 149.91
O 0.3395 110.66
Si 0.000000 0.00
Save every 10000
Random Number Counter 3043887
HELP
Plots
PLOT Window
0 A – 2000 A
Max Target Depth 2000
COLLISION PLOTS
XY Longitudinal
XZ Longitudinal
XY Ions Only
YZ Lateral
All
None
Tile
Clear
Background color White/Black
DISTRIBUTIONS
File Plot
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
HELP
XY Longitudinal
Depth vs. Y-Axis
Si/O2
Silicon
0 A
- Target Depth -
2000 A
Save
Save As
Print
Label
Clear

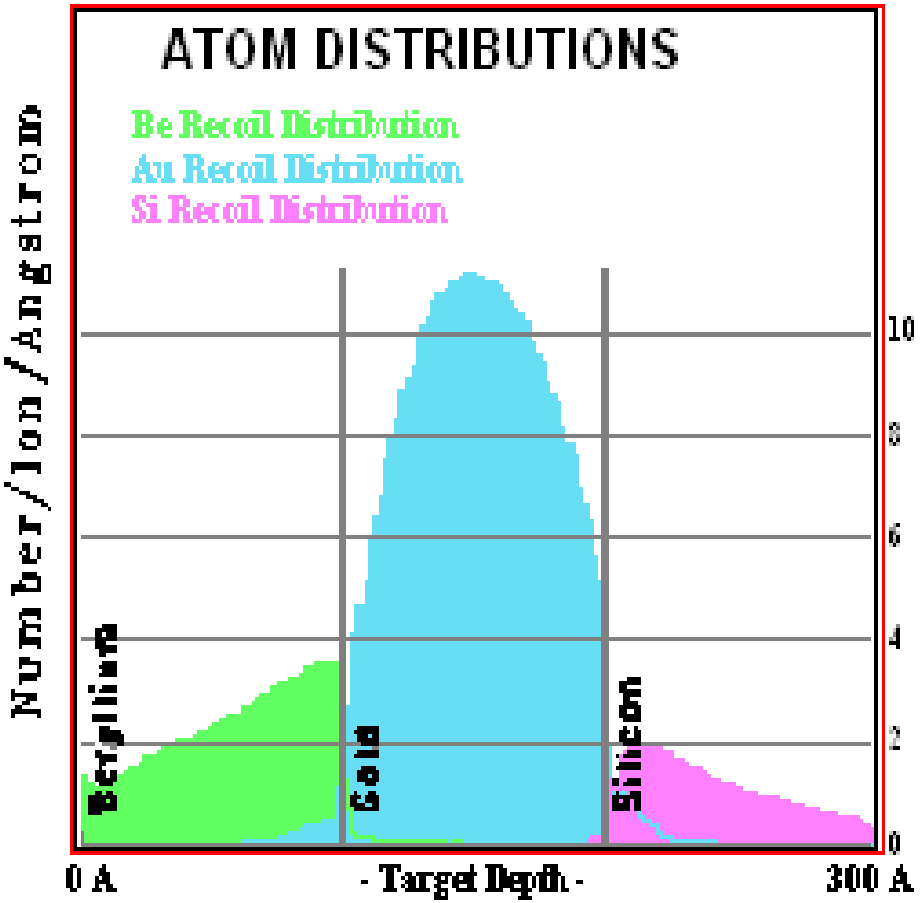
1. Ion distribution



可以看到入射粒子在靶材料中的随深度的最终分布。

离子沉积在它的射程180A 处，存在一个峰值。

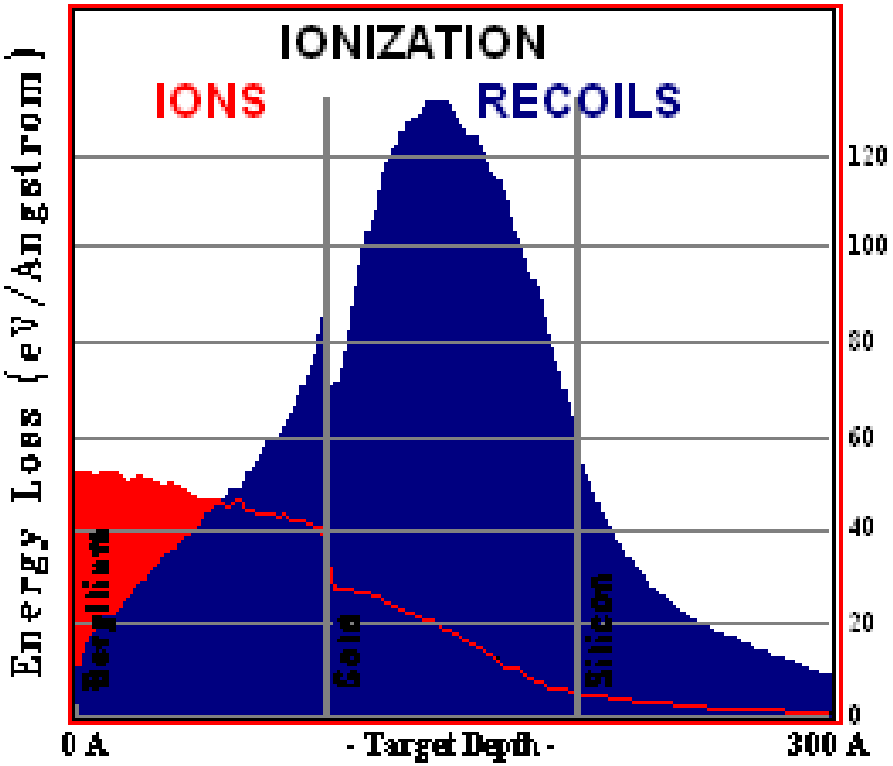
2. recoil distribution
反冲原子的最终分布



左图是U粒子是入射时，靶中级联原子Be、AU、Si的分布情况。

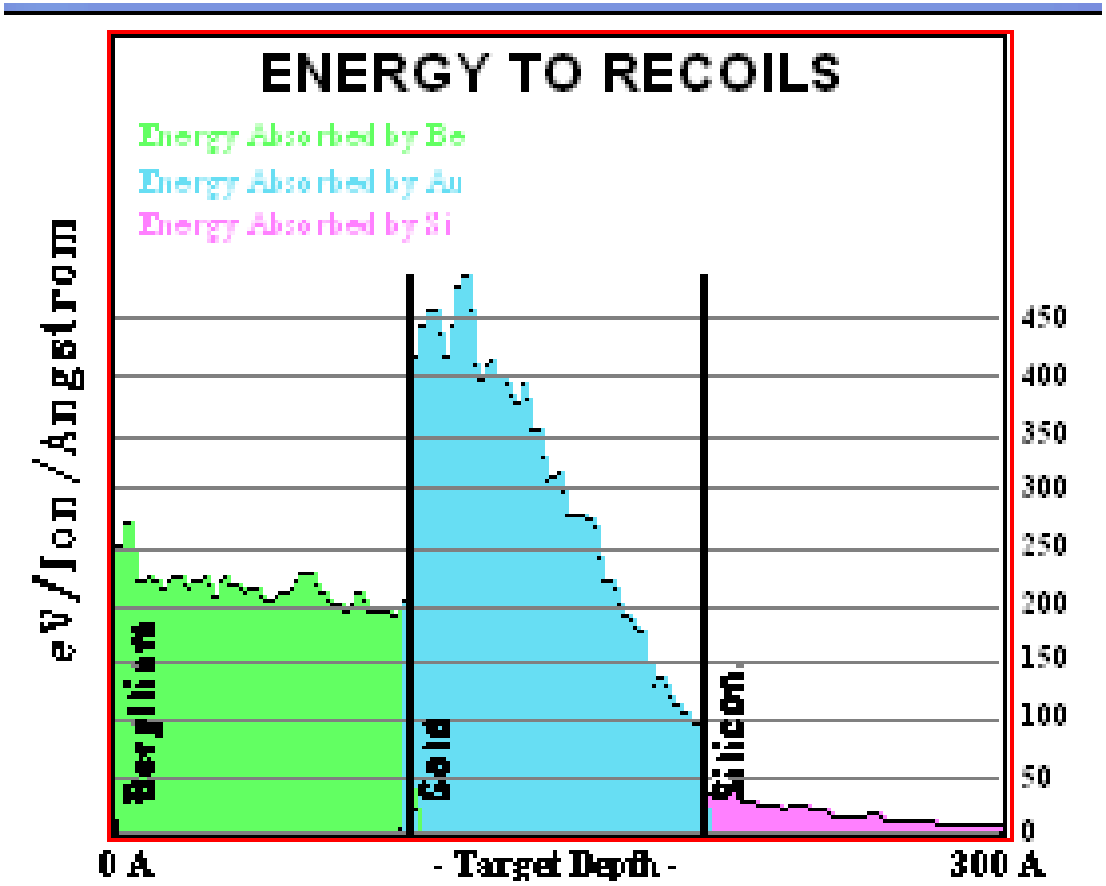
3. ionization

包括两部分：入射粒子和反冲靶原子转移给电子的能量。



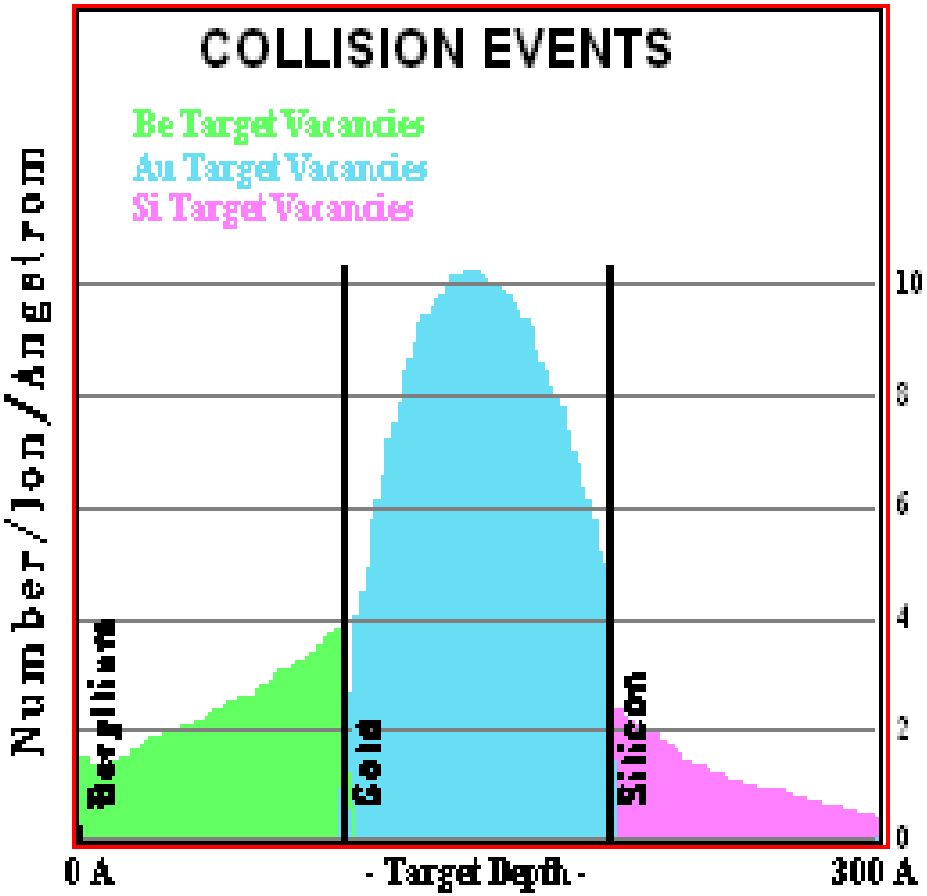
入射离子和级联原子与靶原子核之间发生弹性碰撞，其间并没有能量转化为热能。故靶中总的沉积能量等同于激发、电离电子的能量（电离能损失）。

4. Energy to recoils



5. damage events

- ✓Total displacements
- ✓Total vacancies
- ✓Replacement collisions

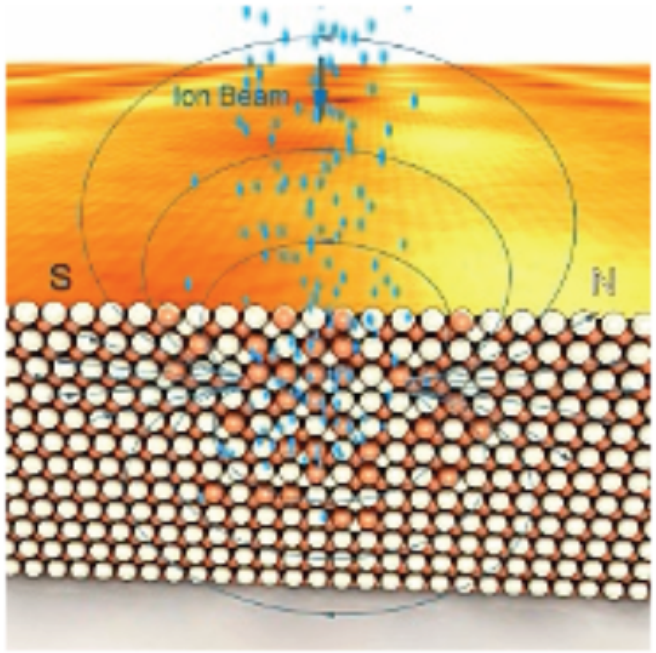


对于每一个入射u粒子来说，在靶中产生总的空位数为1129 个，复位碰撞数105个。总的离位数为1233个。

- Background
- Installing of SRIM
- Introduction of SRIM
- **SRIM Applications**

SRIM Applications

- *Ion Implantation*:
  - Ion beams are used to modify samples by injecting atoms to change the target chemical and electronic properties.
  - The ion beam also causes damage to solid targets by atom displacement.



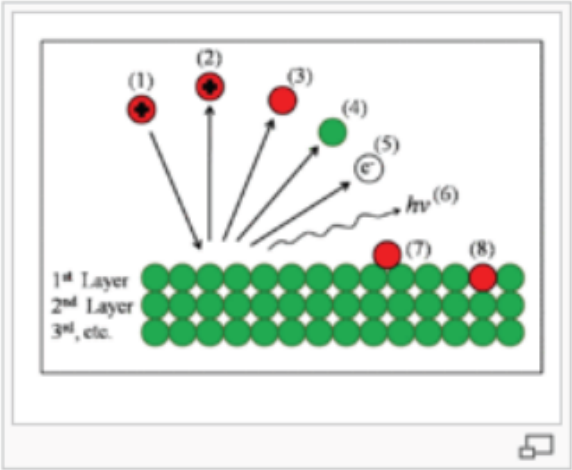
Investigation of phase-change magnonics /magnonics based on ion beam modified materials:

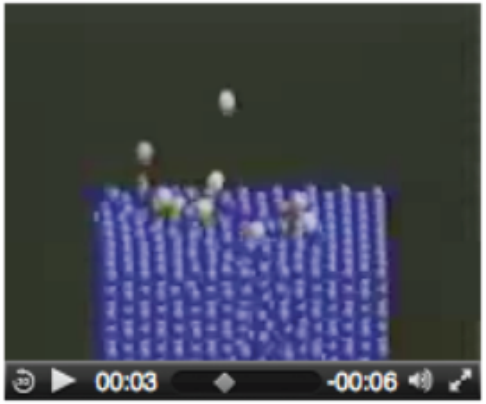
Tailoring of magnetic materials by ion doping:

Courtesy of Prof. Gao at Umich

SRIM Applications

- *Sputtering:*
  - The ion beam may knock out target atoms, a process called *ion sputtering*.





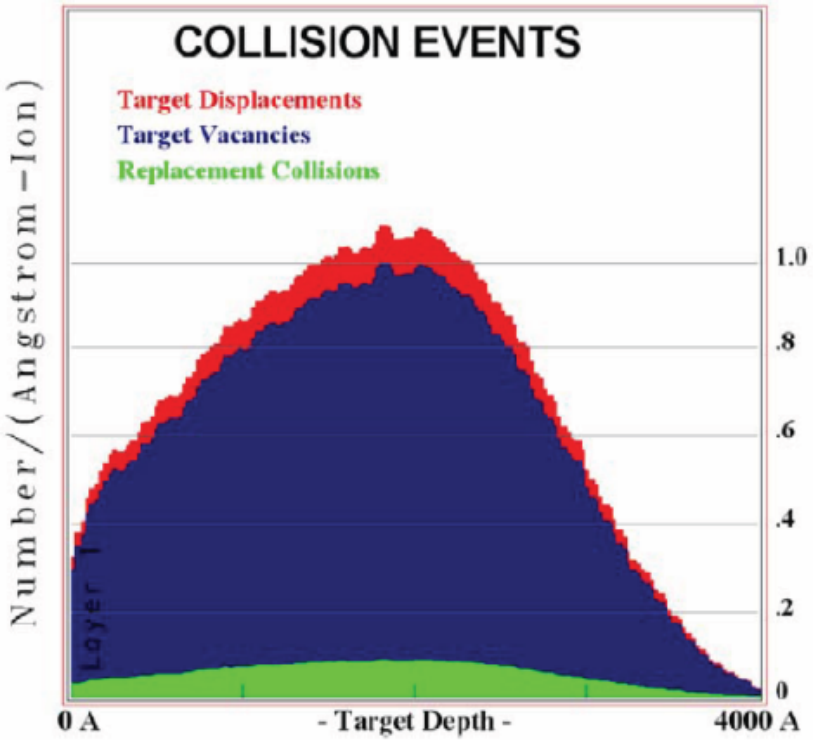
Si^+ - Si (5 keV)

- *Ion Transmission:*
  - Ion beams can be followed through mixed gas/solid target layers, such as occurs in ionization chambers or in energy degrader blocks used to reduce ion beam energies.
- *Ion Beam Therapy:*
  - Ion beams are widely used in medical therapy, especially in radiation oncology.

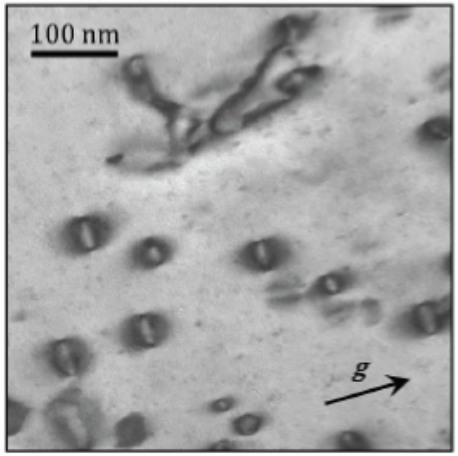
Courtesy of Prof. Gao at Umich

SRIM Applications

- Experimentalists
  - Determine peak damage regime
  - Calculate dpa – radiation damage dose



Peak damage region – important for TEM



Courtesy of Prof. Gao at Umich

Thanks for your attentions!