

# Energy loss of rapid light charged particles in Ion Beam Analysis

présenté par

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# Course Objectives

1. Understand the basic physical approaches and principles involved in theoretical estimations of stopping powers of light ions for IBA
2. Develop a feeling for the main features of the stopping power curve
3. Understand the interplay between theory and data leading to formulation of semi-empirical expressions for stopping powers
4. Know how to use SRIM for stopping power calculations, and critically evaluate the values obtained
5. Acquire basic knowledge of some alternatives to TRIM/SRIM



# Course over-view

Recall of motivation

Interplay between theory and data

Introduction to basic stopping theory

Binary collision model

Electron plasma model

Local density approximation

Bragg's rule, compounds ...

Introduction to TRIM/SRIM

The basic equations

The data files

Accuracy

One or two alternatives :

ICRU 49

Konac

*Based heavily on :*

The Stopping and Range of Ions in Solids. J. F. Ziegler, J. P. Biersack, U. Littmark. Pergamon (1985). ISBN 0-08-021603-X. **'ZBL stopping'**

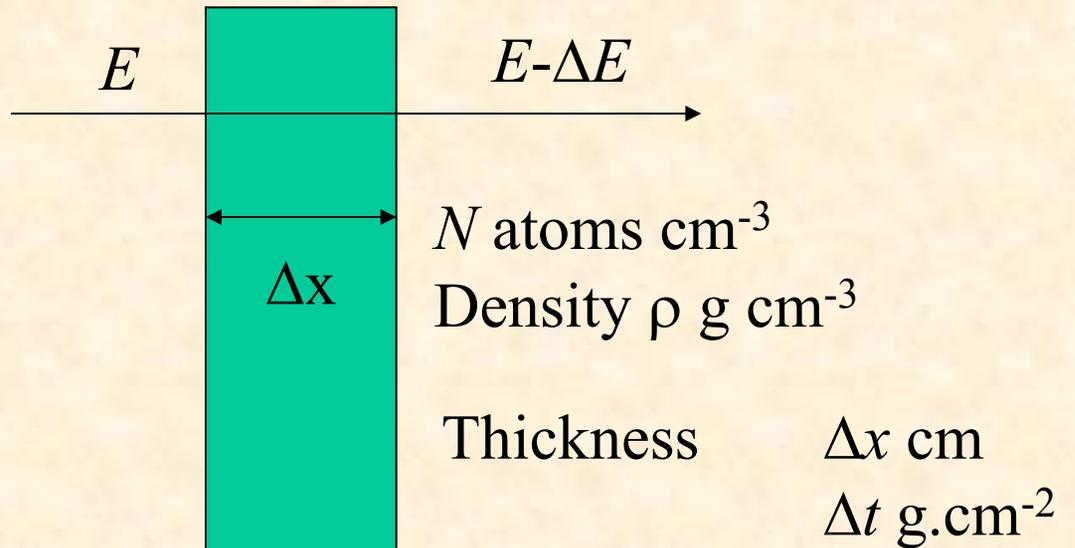
Stopping of energetic light ions in elemental matter. J. F. Ziegler, J. Appl. Phys. 85(3) (1999) 1249-72.



# What is the stopping power?

$$S = \lim_{\Delta x \rightarrow 0} \frac{\Delta E}{\Delta x} = \frac{dE}{dx}$$

Units : eV cm<sup>2</sup> atom<sup>-1</sup>  
 eV cm<sup>2</sup> μg<sup>-1</sup>  
 eV nm<sup>-1</sup>

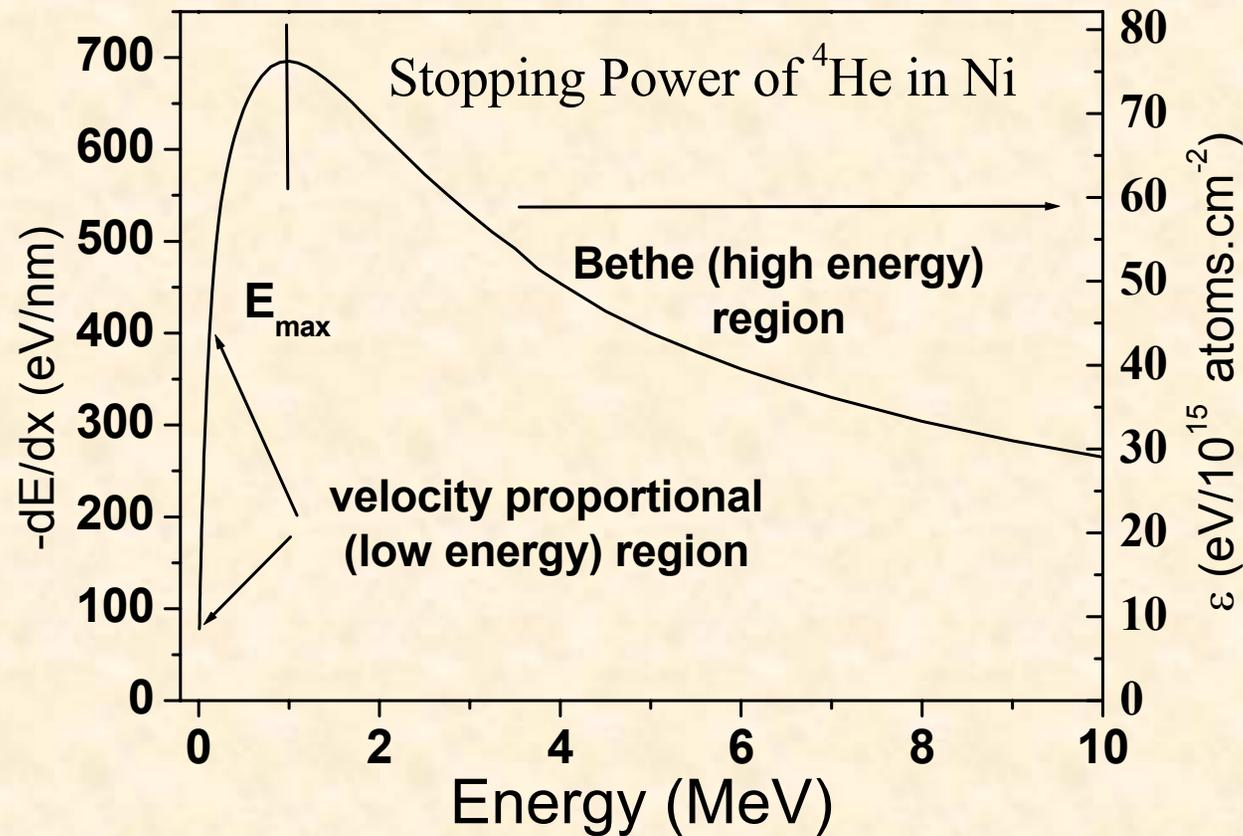


Stopping cross section :  $\varepsilon = -\frac{1}{N} \frac{dE}{dx}$  eVcm<sup>2</sup>

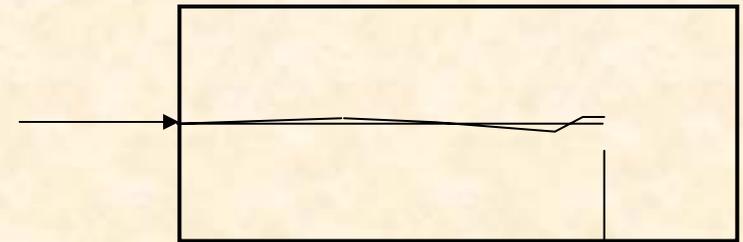
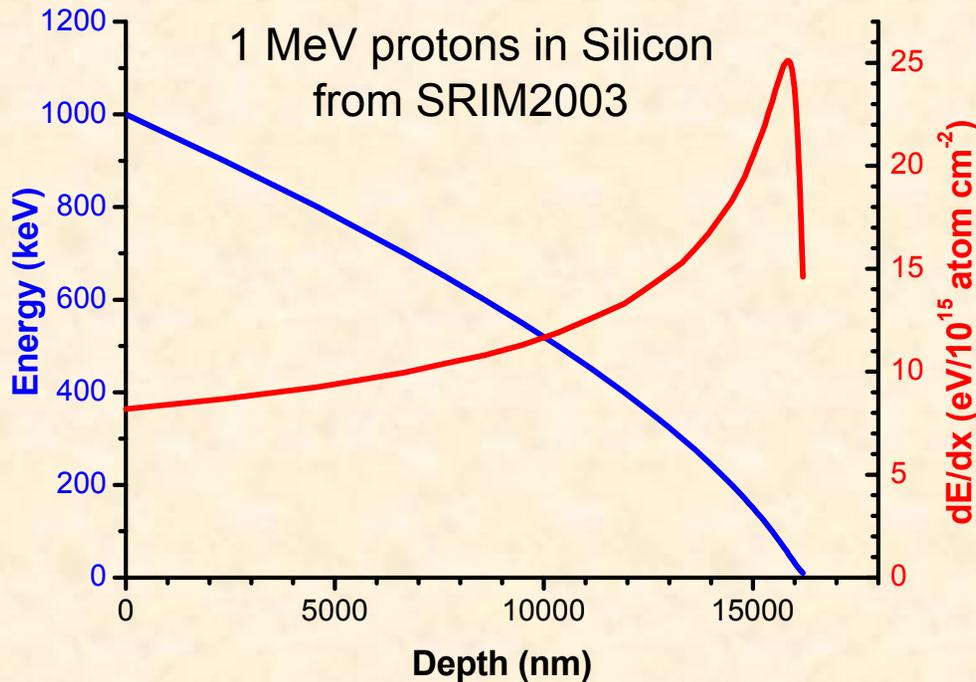
$$t = \rho x$$



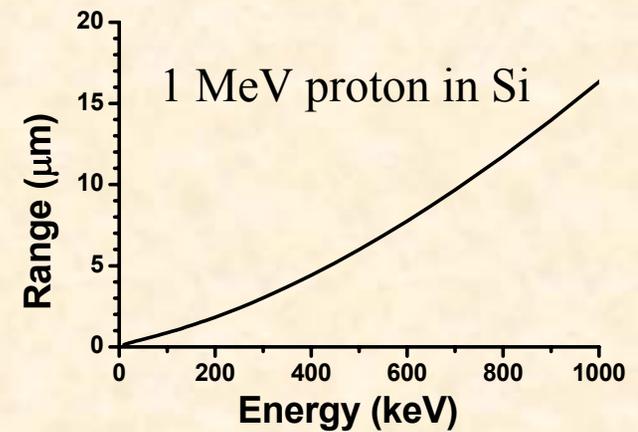
# Basic features of the stopping curve



# Range



$R_p$



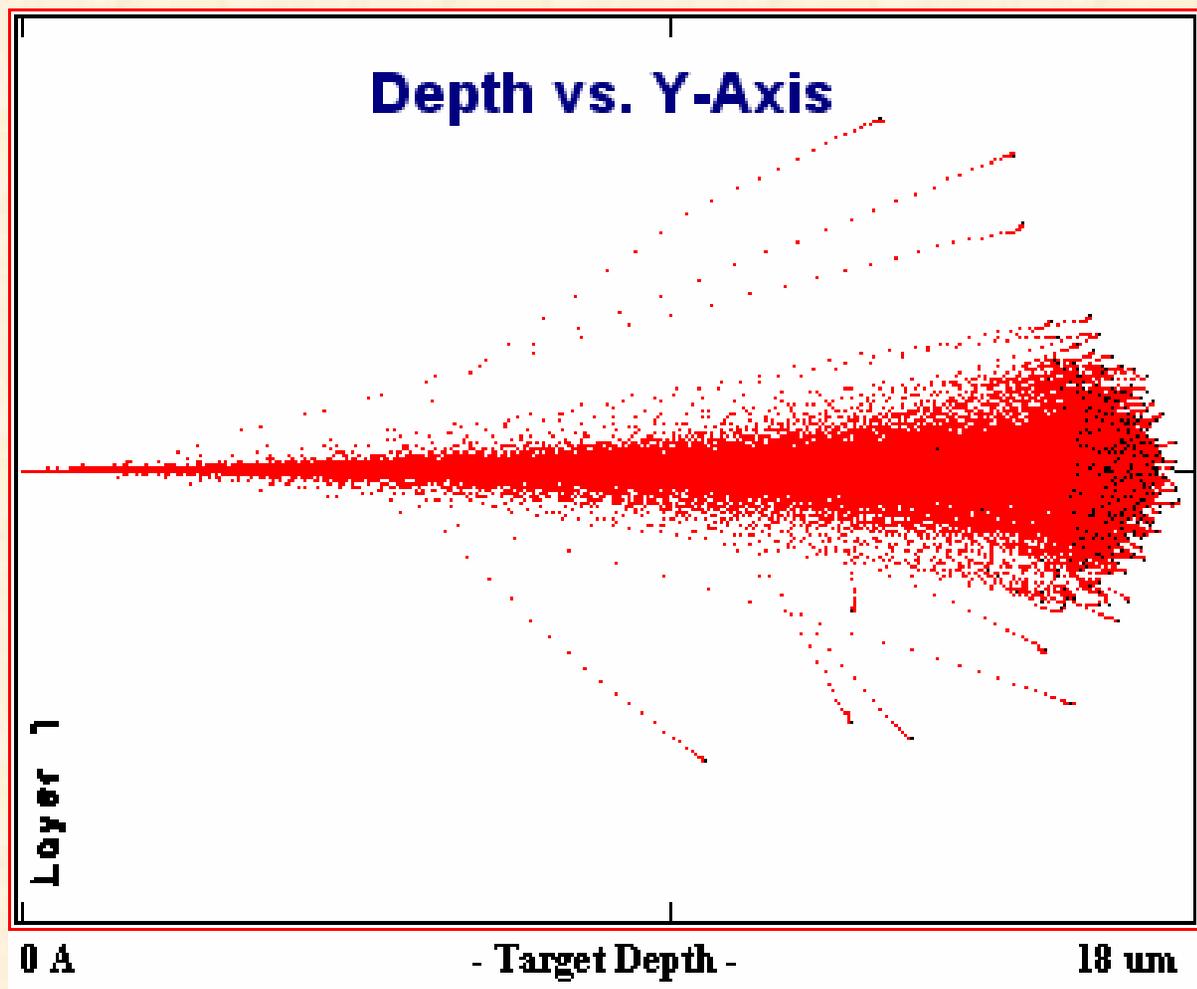
$$R(E) = \int_E^0 \frac{1}{dE/dx} dE = \int_E^0 \frac{1}{S(E)} dE$$

For rapid light ions  
(IBA ...):

$$R_p \approx R$$



# SRIM Monte Carlo calculation



1 MeV protons in Si

2000 incident ions

In this case,

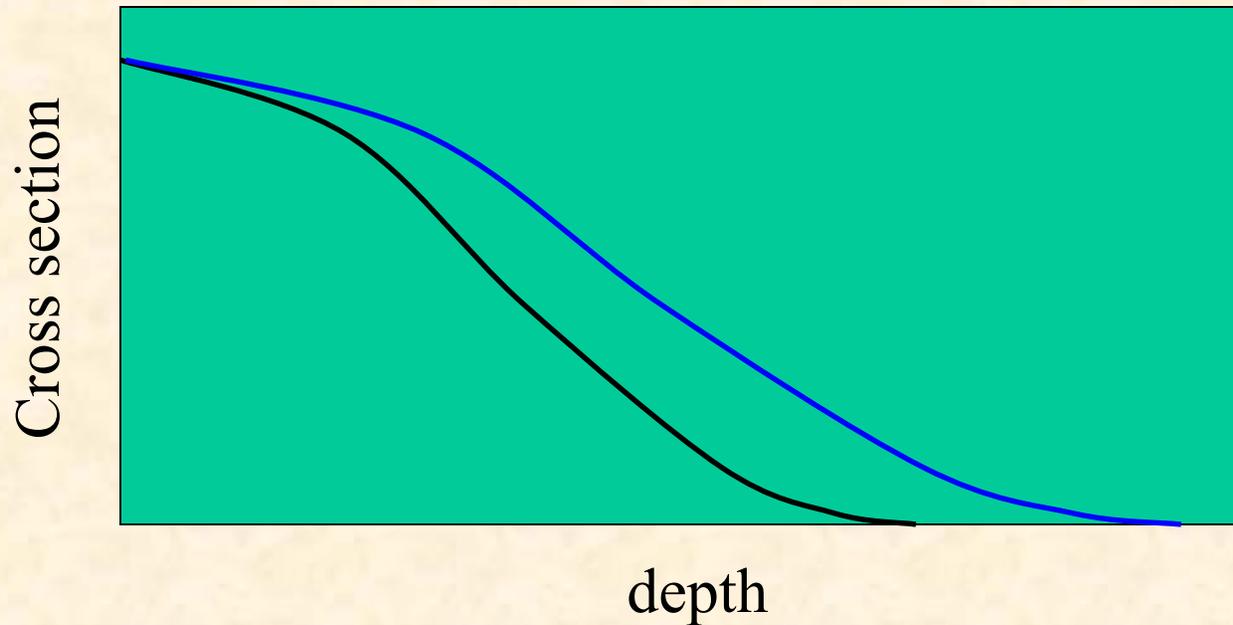
$$\frac{R_p}{R} = 0.98$$

(ICRU report 49)



# Importance of stopping powers in IBA

Thick target PIXE, PIGE

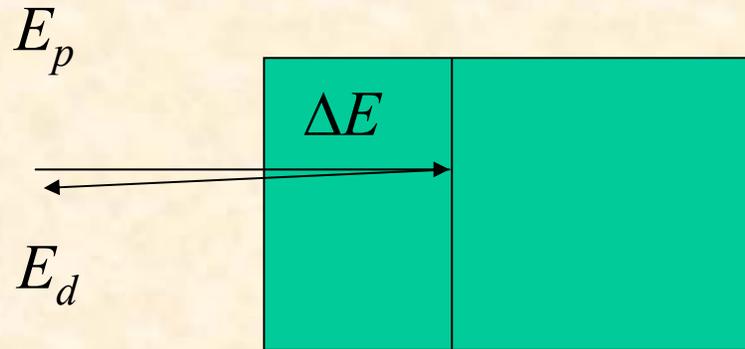


Integrated yields are proportional to range, and so depend on accuracy in stopping powers if different matrices are compared



# Importance of stopping powers in IBA

ERD, RBS, NRA depth profiling



$$E_d = E_p - 2\Delta E$$

$$x = \frac{2\Delta E}{dE/dx}$$

For simplicity, consider RBS on an infinitely heavy target atom at depth  $x$ , and  $\Delta E \ll E_p$

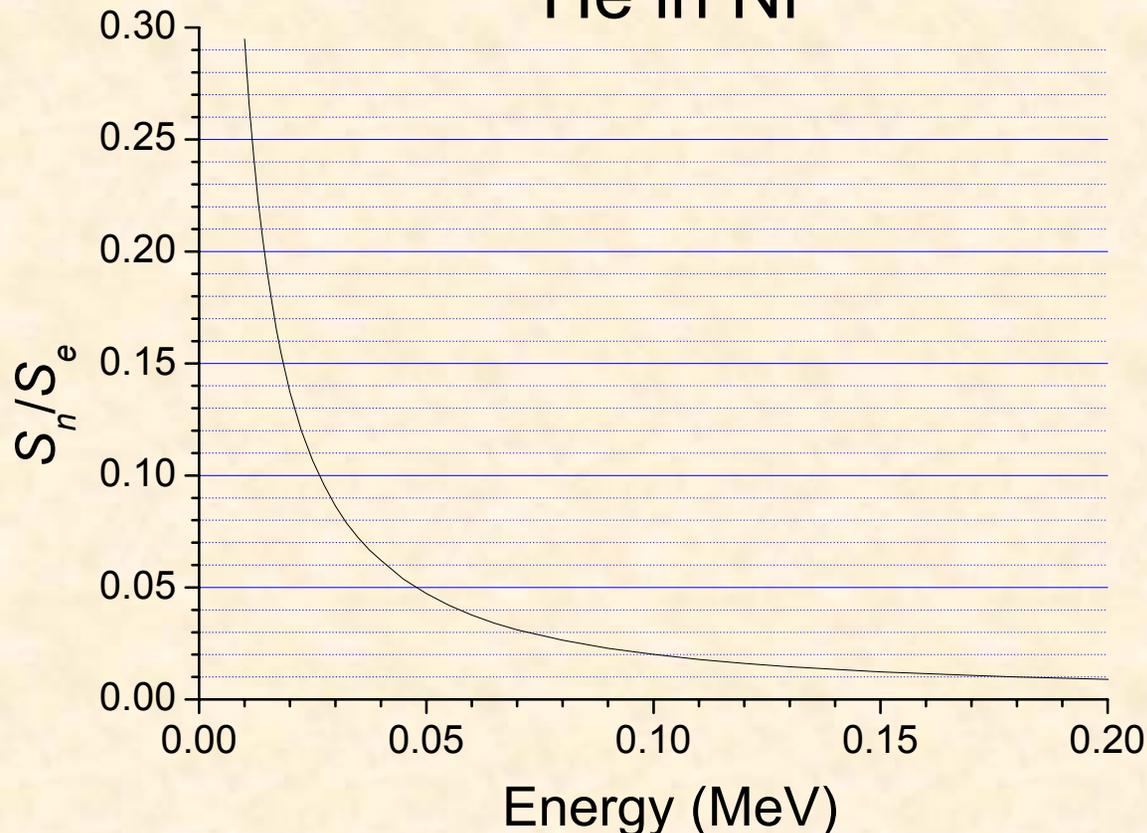
For thick targets, depth scales and spectrum heights are respectively directly and inversely proportional to stopping powers



# Nuclear and electronic stopping

$$S = S_n + S_e$$

$^4\text{He}$  in Ni



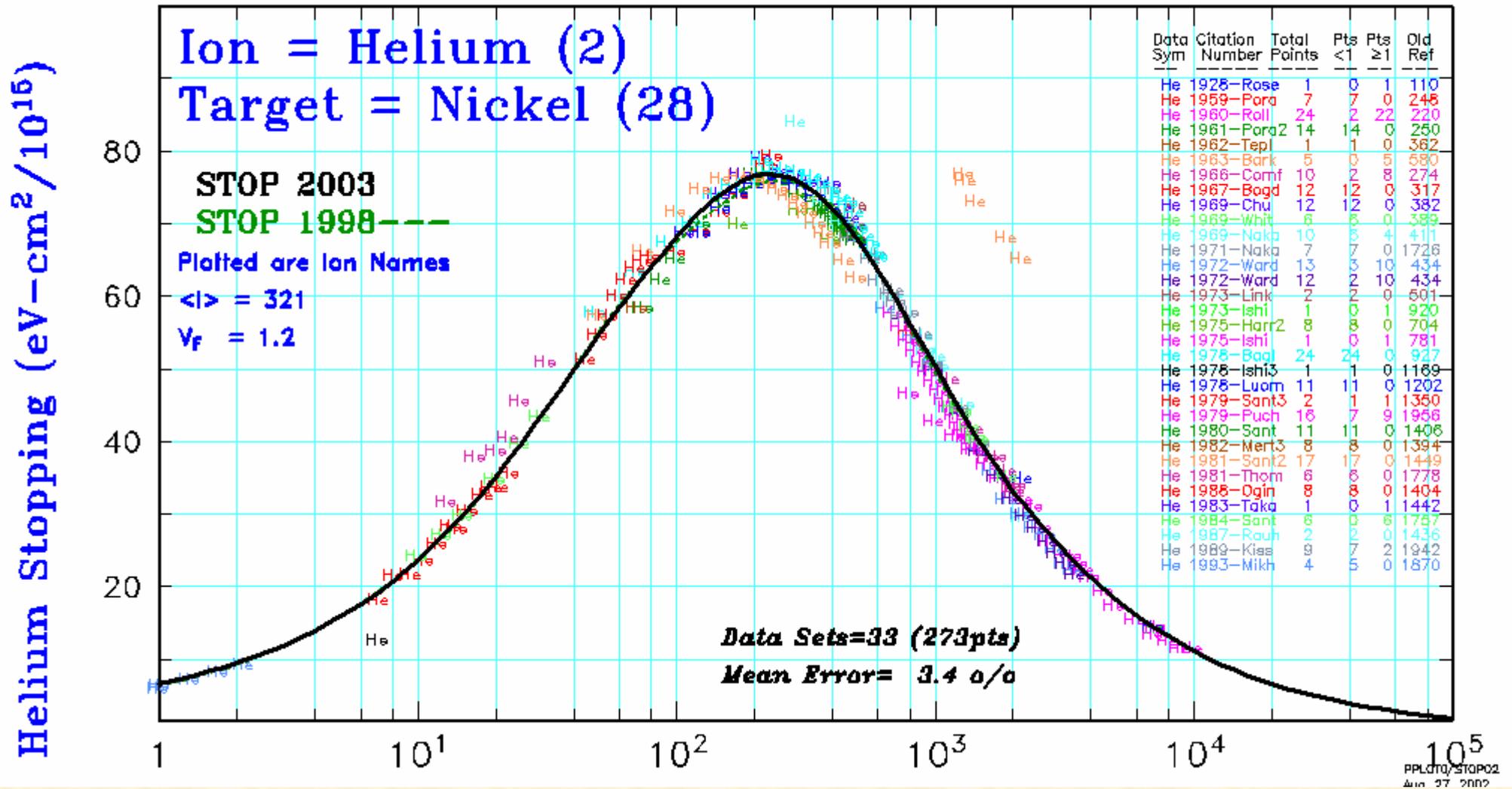
**Nuclear stopping** is due to elastic ion-atom collisions

It is easily calculated from elementary collision physics and may be neglected in the vast majority of IBA measurements.

**Electronic stopping** (sometimes also referred to as inelastic stopping) is due to energy lost to target electrons.

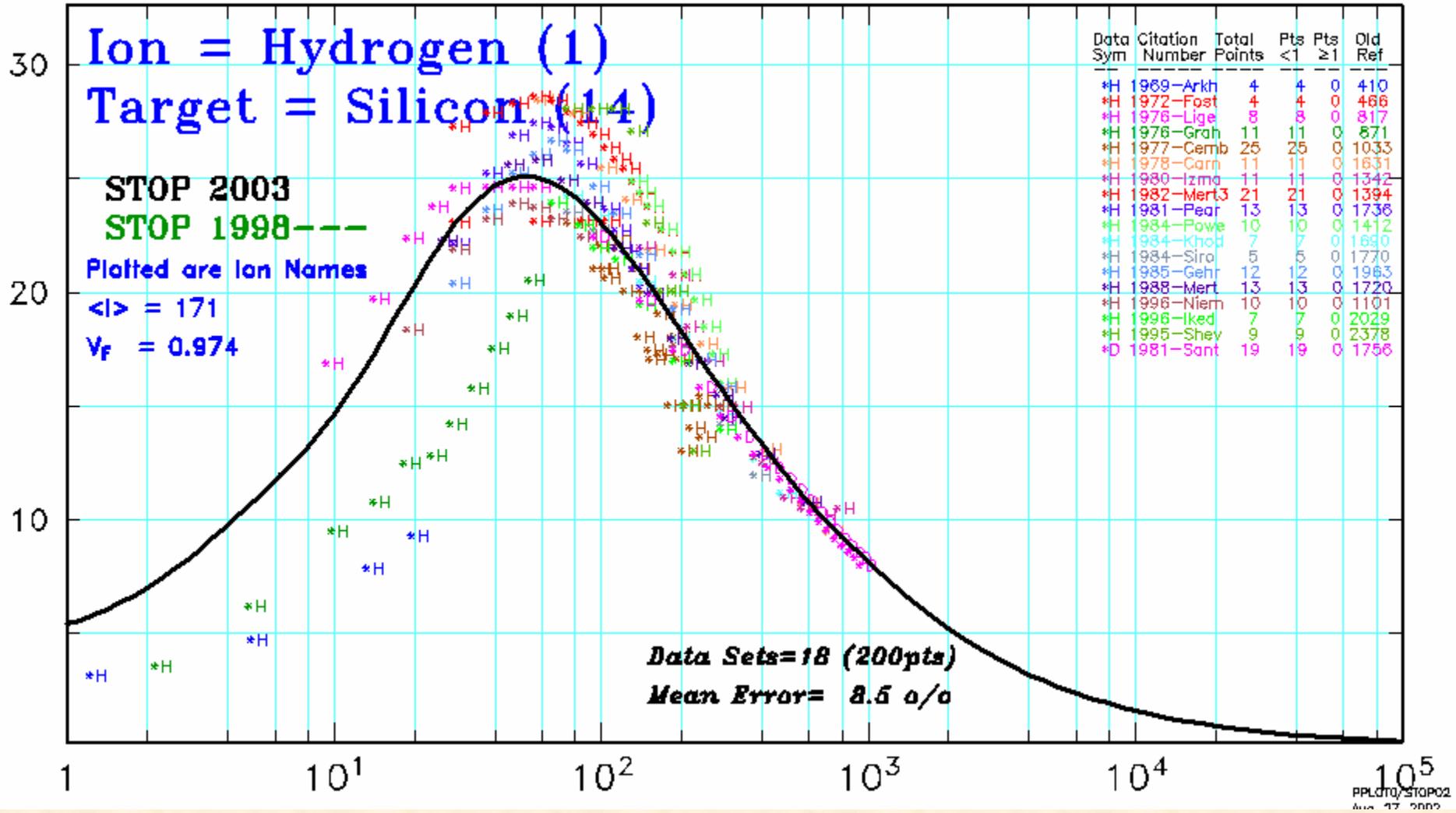


# Real stopping data from SRIM site

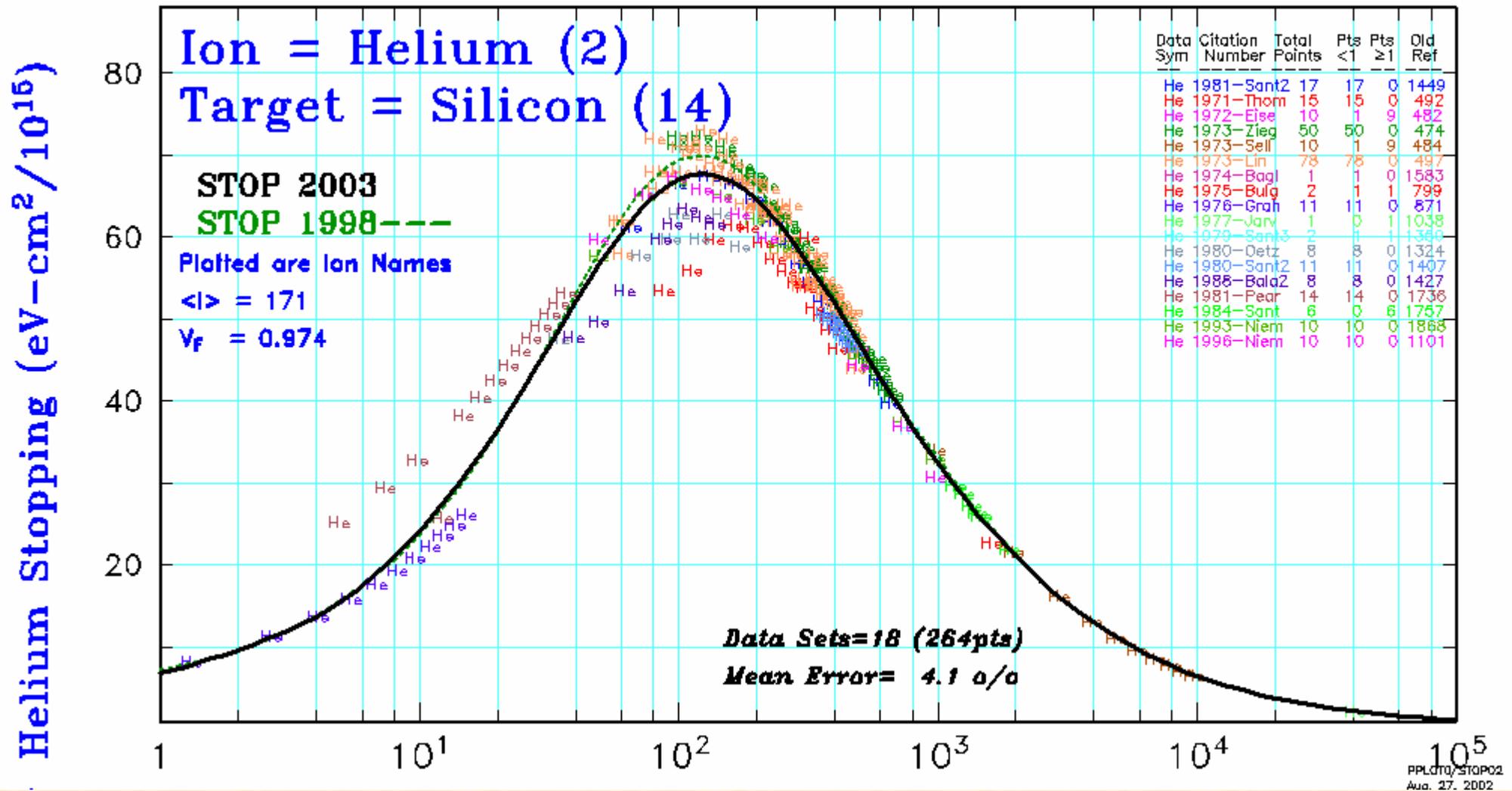


# Protons in silicon

Hydrogen Stopping ( $\text{eV}\cdot\text{cm}^2/10^{16}$ )



# Alphas in silicon



# Basic Stopping Theory

$m$	electron mass
$e$	electron charge
$E$	ion energy
$Z_{1,2}$	ion, target atomic number
$M_{1,2}$	ion, target mass (u)
$v$	ion velocity
$v_0$	Bohr velocity

Bohr - binary ion-electron collisions.  
Target electron binding represented  
by average ionisation energy  $I$ .

Bethe-Bloch. Quantum treatment,  
various correction terms.

Lindhard. Neutral free electron plasma,  
local density approximation.



# Bohr equation

Non-relativistic. Free electrons

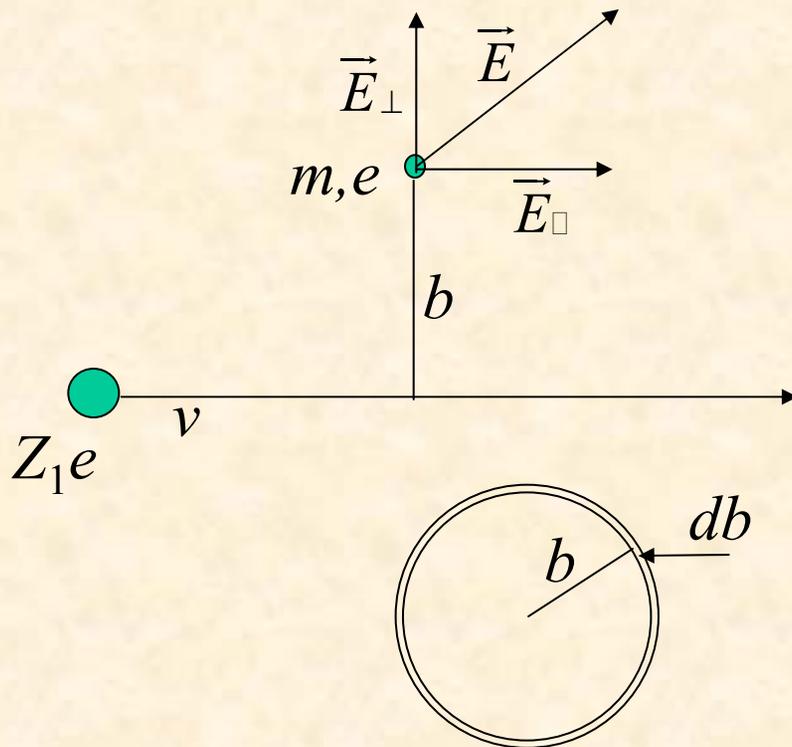
|| momentum impulse = 0

⊥ momentum impulse :

$$\Delta p = \int_{-\infty}^{\infty} e \vec{E}_{\perp}(t) dt = \frac{2Z_1 e^2}{bv}$$

$$\Delta E = \frac{(\Delta p)^2}{2m} = \frac{2Z_1^2 e^4}{mv^2} \left( \frac{1}{b^2} \right)$$

$$\frac{dE}{dx} = 2\pi Z_2 \int \Delta E(b) b db$$



To obtain stopping power per target atom containing  $Z_2$  electrons, integrate over all values of  $b$  :



# Bohr equation

$$\begin{aligned}\frac{dE}{dx} &= 2\pi Z_2 \int \Delta E(b) b db \\ &= 4\pi Z_2 \frac{Z_1^2 e^4}{mv^2} \int_0^\infty \frac{1}{b^2} b db\end{aligned}$$

$$\frac{dE}{dx} = \frac{4\pi e^4 Z_1^2}{mv^2} Z_2 \ln \left( \frac{mv^3}{Z_1 e^2 \omega} \right)$$

$$\frac{dE}{dx} = \frac{4\pi e^4 Z_1^2}{mv^2} Z_2 \ln \left( \frac{2mv^2}{\langle I \rangle} \right)$$

## Integration limits

$b_{min}$  from maximum energy transfer to electron :

$$b_{min} \square \frac{Z_1 e^2}{mv^2}$$

$b_{max}$  from minimum energy transfer to bound electron of orbital frequency  $\omega$ :

$$b_{max} \square \frac{v}{\omega}$$



# (relativistic) Bethe-Bloch equation

$$\frac{dE}{dx} = \frac{4\pi e^4 Z_1^2}{mv^2} Z_2 \left( \ln \frac{2mv^2}{\langle I \rangle} - \ln(1 - \beta^2) - \beta^2 - \frac{C}{Z_2} - \frac{\delta}{2} \right)$$

Target atom mean ionisation energy

Shell correction

Density correction

Stopping number  $L(\beta)$

$$\frac{dE}{dx} = \frac{4\pi e^4 Z_1^2}{mv^2} Z_2 \left[ L_0(\beta) + Z_1 L_1(\beta) + Z_1^2 L_2(\beta) + \dots \right]$$



# Stopping Number

$$L(\beta) = L_0(\beta) + Z_1 L_1(\beta) + Z_1^2 L_2(\beta) + \dots$$

Barkas term

Bloch correction

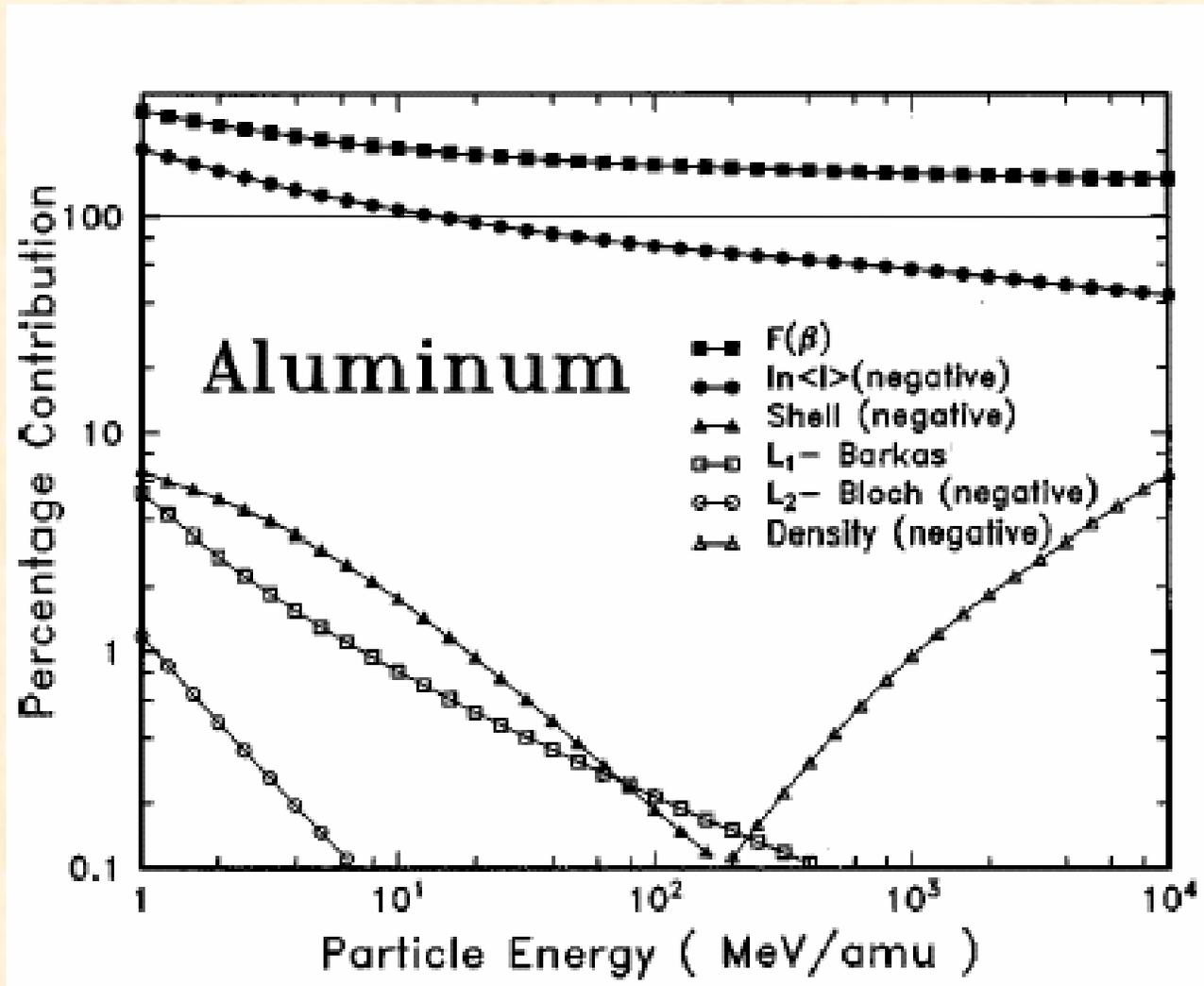
$$L_0(\beta) = \ln\left(\frac{2mc^2\beta^2}{1-\beta^2}\right) - \beta^2 \frac{C}{Z_2} - \ln\langle I \rangle - \frac{\delta}{2}$$

Shell correction      Density correction



# Relative contributions of the different terms

Protons in Al.



# Lindhard theory

## Free electron plasma

$$S_e = \int I(v, \rho) Z_1^2 \rho dV$$

↑  
Interaction function

$I\rho$  is called the stopping integrand

$$I(v, \rho) = \frac{4\pi e^4}{mv^2} \frac{i}{\pi\omega_0^2} \int_0^\infty \frac{dk}{k} \int_{-kv}^{kv} \omega d\omega \left[ \frac{1}{\varepsilon^l(k, \omega)} - 1 \right]$$

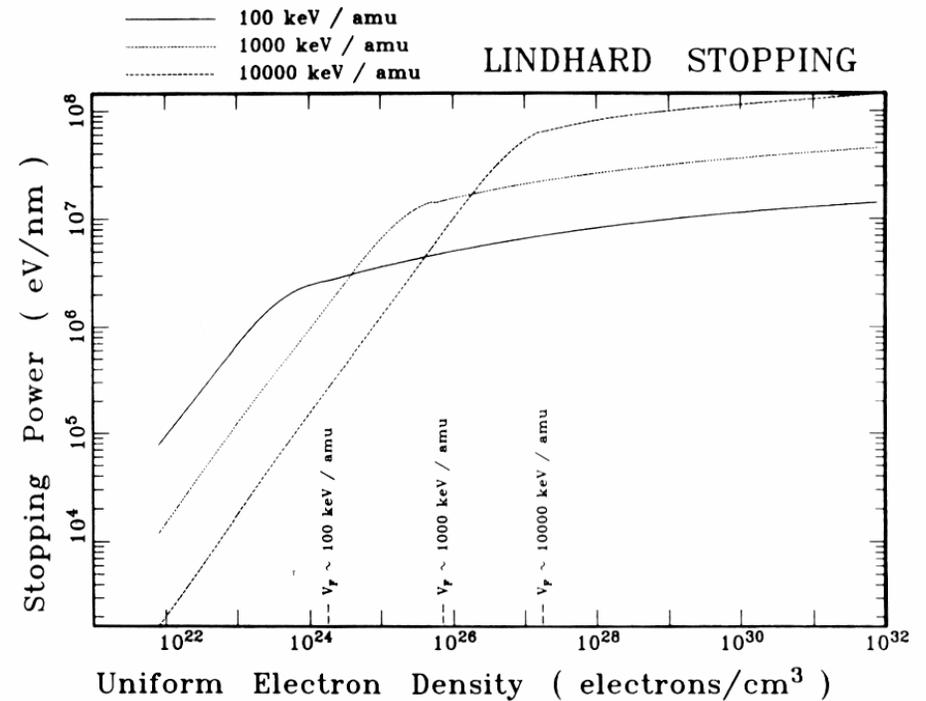
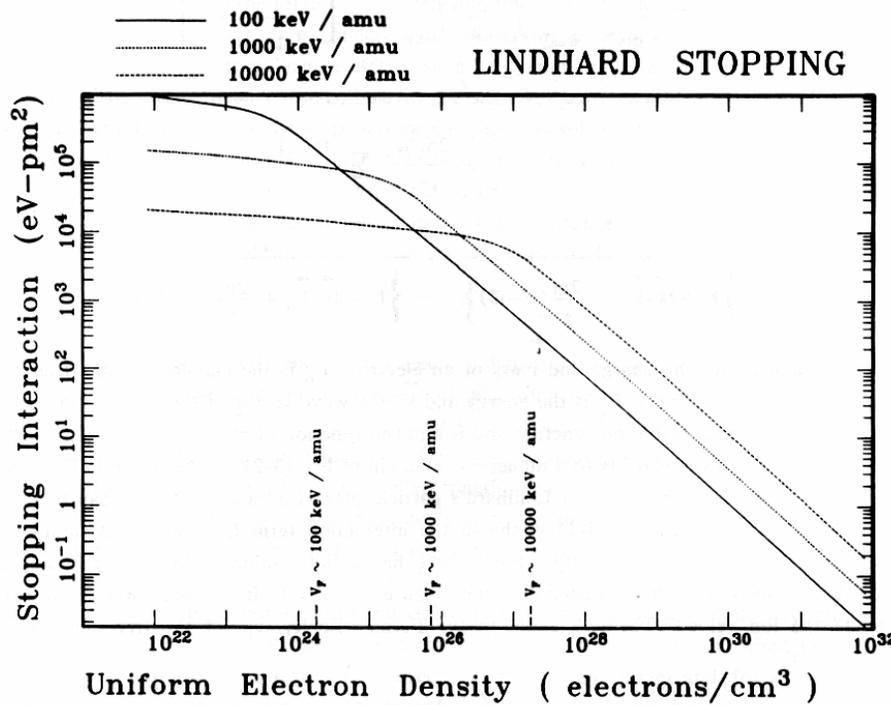
$$Z_2 = \int_{\text{atomic volume}} \rho dV$$



# Values of $I$ and $I\rho$

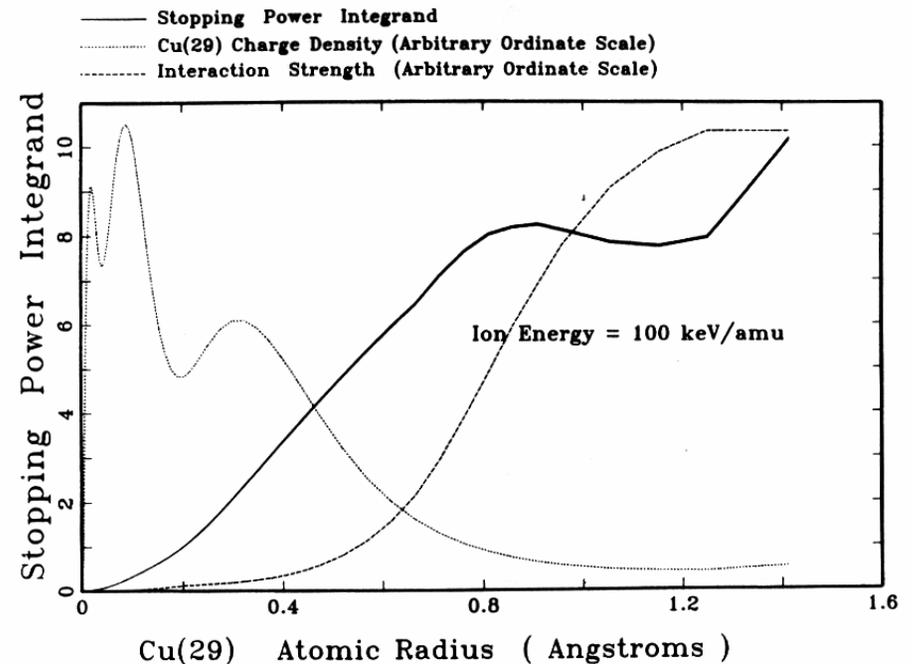
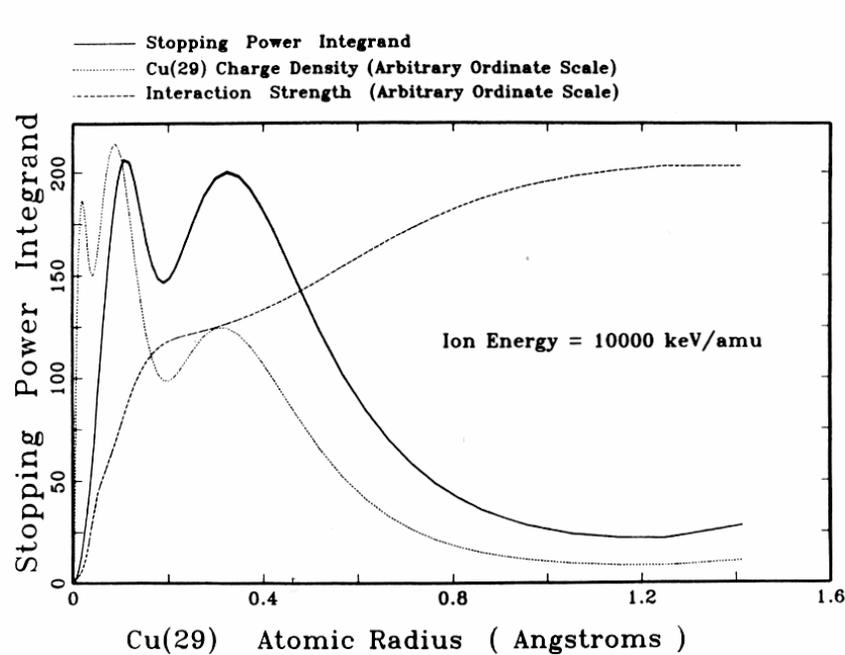
$$I(v,\rho)$$

$$\rho I(v,\rho)$$



# Local Density Approximation

Use electron densities  $\rho(\vec{r})$  deduced from atomic models, and assume that the electrons behave locally as a free electron gas. Sum (integrate) over  $\vec{r}$

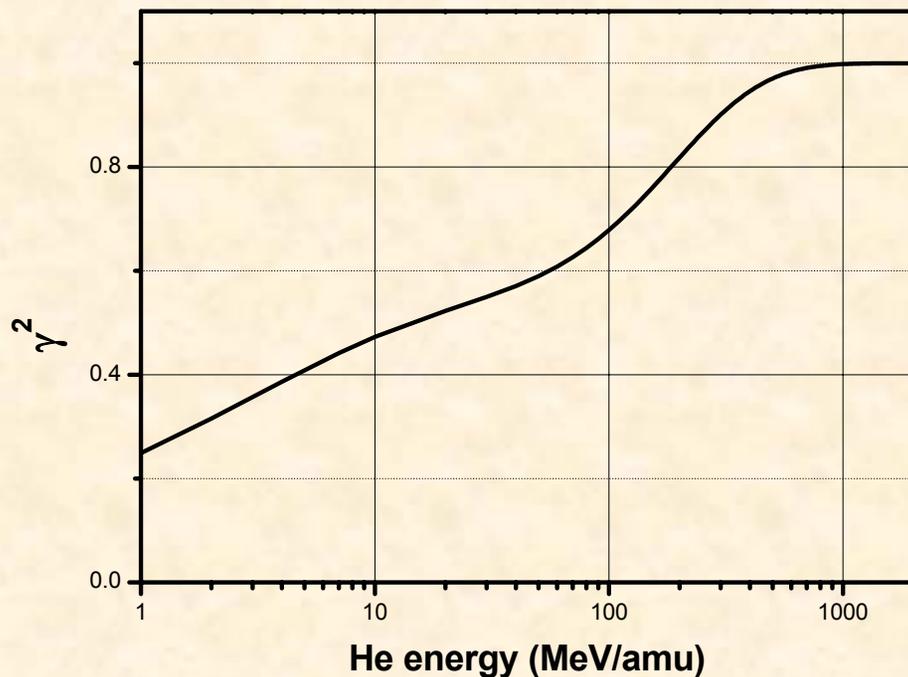


# Effective charge

Protons (and deuterons ...) are always completely stripped.

For He ions we define  $Z_{\text{eff}} = \gamma Z_{\text{He}}$

Ziegler finds :



$$\gamma_{\text{He}}^2 = 1 - e^{\left[ -\sum_0^5 a_i \ln(E)^i \right]}$$

$a_0$	0.2865
$a_1$	0.1266
$a_2$	-0.001429
$a_3$	0.2402
$a_4$	-0.1135
$a_5$	0.001475



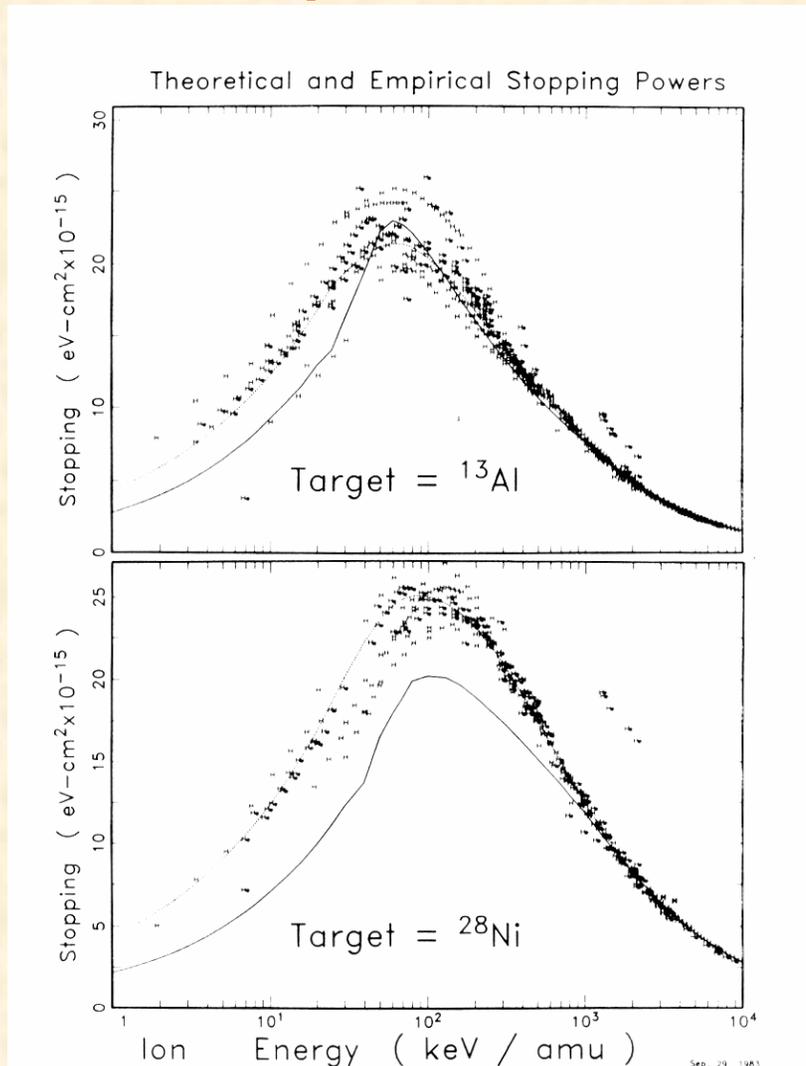
## Scaling rule

$$\left. \begin{aligned} S_e &= \int I(v, \rho) Z_1^2 \rho dV \\ \frac{dE}{dx} &= \frac{4\pi e^4 Z_1^2}{mv^2} Z_2 \ln \left( \frac{2mv^2}{\langle I \rangle} \right) \end{aligned} \right\} S_e \propto Z_1^2$$

$$S_e^{He}(v) = 4\gamma^2 S_e^H(v)$$



# Comparison of Lindhard theory and data



For protons and helium ions :

Above about 1 MeV/amu, theory looks ok

Discrepancies up to 20-30% below 1MeV/amu.

Use an effective proton charge  $\chi(v)$  for protons, fitted by using data for all targets. This is an empirical correction factor.



# Low energy stopping power

$v < v_B$

$v_B$  is velocity of electron in first hydrogen orbit :  
 $c/137$  or 25 keV/amu

Lindhard, Scharff, Schiot (LSS) stopping :

$$S_e(E) \propto \frac{Z_1^{7/6} Z_2}{\left( Z_1^{2/3} + Z_2^{2/3} \right)^{3/2}} E^s$$

$S=1/2$  -> 'velocity proportional regime'



# Semi-empirical models for elemental stopping powers of protons

The game consists of finding a universal formula, which converges to the Bethe-Bloch or Lindhard form for high energies and to the velocity-dependant form at low energies, and then adjusting fit parameters to best represent reliable experimental values.

By far the most widely known and used is that proposed by ZBL and updated in TRIM and SRIM programs by Ziegler.



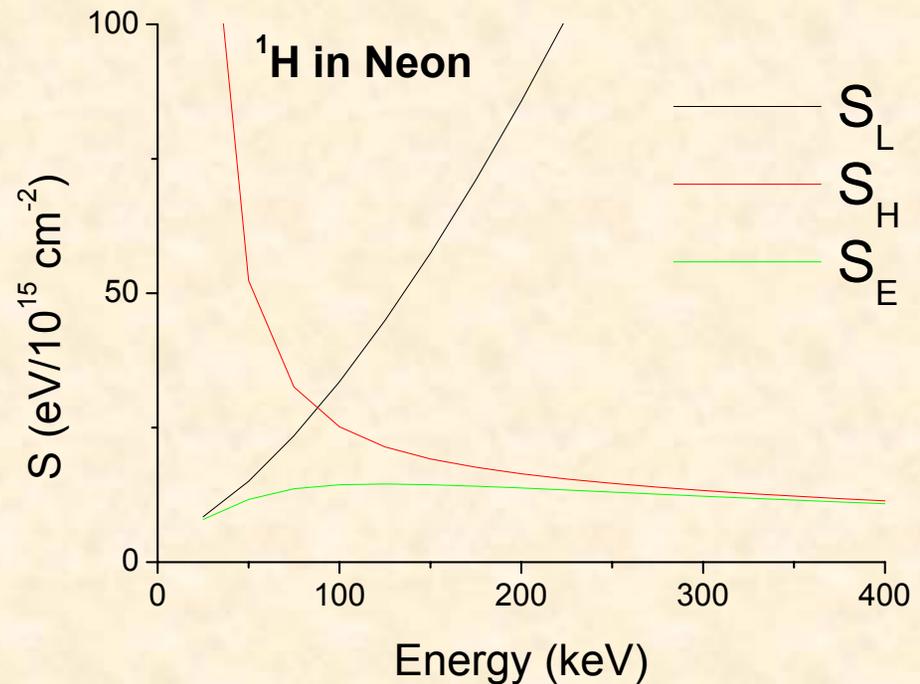
# The basic TRIM formulae for protons

[www.srim.org](http://www.srim.org), <http://www.nea.fr/abs/html/nea-0919.html>

$$S_E = \frac{S_L S_H}{S_L + S_H}$$

$$S_L = aE^b + cE^d$$

$$S_H = e \frac{\ln\left(\frac{g}{E} + hE\right)}{E^f}$$



## Values of coefficients

$$S_L = aE^b + cE^d$$

$$S_H = e \frac{\ln\left(\frac{g}{E} + hE\right)}{E^f}$$

a	2.072
b	0.0044516
c	3.5585
d	0.53933
e	1515.2
f	0.93161
g	1790.3
h	0.035198

Values for protons in silicon, from  
SCOEF.ASC, published in ZBL vol 1  
1985



File : SCOE DATA (Contains data on elemental ions and solids)

\*\*\*\* Comments on this file. Do not include in computer data file.

ROWS 1 - 92:

Column #1 = Atomic Number  
 Column #2 = Atomic Mass of most abundant isotope  
 Column #3 = Atomic weight of most abundant isotope  
 Column #4 = Atomic weight of solid with normal isotopic abundance  
 Column #5 = Density of solid in grams/cm<sup>3</sup>  
 Column #6 = Density of solid in units of 1E22 atoms/cm<sup>3</sup>  
 Column #7 = Fermi velocity of solid, in units of the Bohr velocity  
 Column #8 = Factor determining ion screening length

ROWS 93 - 184

Column #1 = Atomic Number  
 Columns #2-9 = Proton stopping cross-section coefficients

-----  
SCOE DATA : VERSION - 1985  
-----

1	1	1.0078	1.008	0.071486	4.271	1.0309	1.
2	4	4.0026	4.0026	0.12588	1.894	0.15976	1.
3	7	7.016	6.939	0.52969	4.597	0.59782	1.1
4	9	9.012	9.0122	1.8024	12.046	1.0781	1.06
5	11	11.009	10.811	2.3502	13.093	1.0486	1.01
6	12	12.	12.011	2.2662	11.364	1.	1.03
7	15	14.003	14.007	0.80963	3.481	1.058	1.04
8	16	15.995	15.999	1.1429	4.302	0.93942	0.99
9	19	18.998	18.998	1.1111	3.522	0.74562	0.95
10	20	19.992	20.183	1.2015	3.585	0.3424	0.9
11	23	22.99	22.989	0.97	2.541	0.45259	0.82
12	24	23.985	24.312	1.7366	4.302	0.71074	0.81
13	27	26.982	26.981	2.6981	6.023	0.90519	0.83
14	28	27.977	28.086	2.3212	4.977	0.97411	0.88
15	31	30.994	30.973	1.8219	3.542	0.97184	1.
16	32	31.97	32.064	2.0686	3.885	0.89852	0.95
17	35	34.969	35.453	1.8956	3.22	0.70827	0.97
18	40	39.98	39.948	1.6504	2.488	0.39816	0.99
19	39	38.96	39.102	0.86318	1.329	0.36552	0.98
20	40	39.96	40.08	1.54	2.014	0.62712	0.97
21	45	44.956	44.956	2.9971	4.015	0.81707	0.98
22	48	47.95	47.9	4.5189	5.682	0.9943	0.97
23	51	50.94	50.942	6.1008	7.213	1.1423	0.96
24	52	51.94	51.996	7.1917	8.33	1.2381	0.93
25	55	54.94	54.938	7.4341	8.15	1.1222	0.91
26	56	55.94	55.847	7.8658	8.483	0.92705	0.9
27	59	58.93	58.933	8.796	8.989	1.0047	0.88
28	58	57.94	58.71	8.8955	9.125	1.2	0.9
29	63	62.93	63.54	8.9493	8.483	1.0661	0.9
30	64	63.93	65.37	7.1054	6.546	0.97411	0.9
31	69	68.93	69.72	5.9085	5.104	0.84912	0.9
32	74	73.92	72.59	5.3375	4.428	0.95	0.85
33	75	74.92	74.922	5.7192	4.597	1.0903	0.9
34	80	79.92	78.96	4.7855	3.65	1.0429	0.9
35	79	78.92	79.909	3.3995	2.562	0.49715	0.91
36	84	83.92	83.8	2.6021	1.87	0.37755	0.92
37	85	84.91	85.47	1.529	1.077	0.35211	0.9
38	88	87.91	87.62	2.6	1.787	0.57801	0.9
39	90	89.91	88.905	4.4902	3.041	0.77773	0.9
40	90	89.9	91.22	6.4695	4.271	1.0207	0.9
41	93	92.91	92.906	8.6024	5.576	1.029	0.9

42	96	95.5	95.94	10.206	6.407	1.2542	0.88	
43	0	0.	99.	0.	0.	1.122	0.9	
44	102	101.9	101.07	12.177	7.256	1.1241	0.88	
45	103	102.9	102.91	12.399	7.256	1.0882	0.88	
46	106	105.9	106.4	11.955	6.767	1.2709	0.9	
47	107	106.9	107.87	10.473	5.847	1.2542	0.9	
48	114	113.9	112.4	8.5802	4.597	0.90094	0.88	
49	115	114.9	114.82	7.3134	3.836	0.74093	0.9	
50	120	119.9	118.69	7.2816	3.695	0.86054	0.9	
51	121	120.9	121.75	6.6168	3.273	0.93155	0.9	
52	130	130.	127.6	6.2244	2.938	1.0047	0.9	
53	127	126.9	126.9	4.9373	2.343	0.55379	0.96	
54	130	129.5	131.3	3.0589	1.403	0.43289	1.2	
55	134	134.	132.91	1.8986	0.86	0.32636	0.9	
56	138	138.	137.34	3.5215	1.544	0.5131	0.88	
57	139	139.	138.91	6.1738	2.676	0.695	0.88	
58	140	140.	140.12	6.6724	2.868	0.72591	0.85	
59	141	141.	140.91	6.7744	2.895	0.71202	0.9	
60	142	142.	144.24	7.0019	2.923	0.67413	0.9	
61	0	0.	147.	0.	0.	0.71418	0.92	
62	152	152.	150.35	7.5553	3.026	0.71453	0.95	
63	153	153.	151.96	5.2581	2.084	0.5911	0.99	
64	158	157.9	157.25	7.902	3.026	0.70263	1.03	
65	160	159.9	158.92	8.2773	3.136	0.68049	1.05	
66	164	164.	162.5	8.5526	3.17	0.68203	1.07	
67	165	165.	164.93	8.8198	3.22	0.68121	1.08	
68	166	166.	167.26	9.0902	3.273	0.68532	1.1	
69	169	169.	168.93	9.3331	3.327	0.68715	1.08	
70	174	174.	173.04	6.9774	2.428	0.61884	1.08	
71	175	175.	174.97	9.8298	3.383	0.71801	1.08	
72	180	180.	178.49	13.124	4.428	0.83048	1.08	
73	181	181.	180.95	16.601	5.525	1.1222	1.09	
74	184	184.	183.85	19.292	6.32	1.2381	1.09	
75	187	187.	186.2	21.04	6.805	1.045	1.1	
76	192	192.	190.2	22.562	7.144	1.0733	1.11	
77	193	193.	192.2	22.506	7.052	1.0953	1.12	
78	195	195.	195.09	21.438	6.618	1.2381	1.13	
79	197	197.	196.97	19.311	5.904	1.2879	1.14	
80	202	202.	200.59	13.553	4.069	0.78654	1.15	
81	205	205.	204.37	11.882	3.501	0.66401	1.17	
82	208	208.	207.19	11.322	3.291	0.84912	1.2	
83	209	209.	208.98	9.8113	2.827	0.88433	1.18	
84	210	210.	210.	9.2511	2.653	0.80746	1.17	
85	210	210.	210.	0.	0.	0.43357	1.17	
86	222	222.	222.	0.	0.	0.41923	1.16	
87	223	223.	223.	0.	0.	0.43638	1.16	
88	226	226.	226.	5.0222	1.338	0.51464	1.16	
89	227	227.	227.	0.	0.	0.73087	1.16	
90	232	232.	232.	11.658	3.026	0.81065	1.16	
91	231	231.	231.	15.4	4.015	1.9578	1.16	
92	238	238.04	238.04	19.043	4.818	1.0257	1.16	
1	0.0091827	0.0053496	0.69741	0.48493	316.07	1.0143	9329.3	0.053989
2	0.11393	0.0051984	1.0822	0.39252	1081.	1.0645	4068.5	0.017699
3	0.85837	0.0050147	1.6044	0.38844	1337.3	1.047	2659.2	0.01898
4	0.8781	0.0051049	5.4232	0.2032	1200.6	1.0211	1401.8	0.038529
5	1.4608	0.0048836	2.338	0.44249	1801.3	1.0352	1784.1	0.02024
6	3.2579	0.0049148	2.7156	0.36473	2092.2	1.0291	2643.6	0.018237
7	0.59674	0.0050837	4.2073	0.30612	2394.2	1.0255	4892.1	0.016006
8	0.75253	0.0050314	4.0824	0.30067	2455.8	1.0181	5069.7	0.017426
9	1.226	0.0051385	3.2246	0.32703	2525.	1.0142	7563.6	0.019469
10	1.0332	0.0051645	3.004	0.33889	2338.6	0.99997	6991.2	0.021799

Table from file  
 SCOE.DAT  
 used in  
 TRIM85



11	6.0972	0.0044292	3.1929	0.45763	1363.3	0.95182	2380.6	0.081835
12	14.013	0.0043646	2.2641	0.36326	2187.4	0.99098	6264.8	0.0462
13	0.039001	0.0045415	5.5463	0.39562	1589.2	0.95316	816.16	0.047484
14	2.072	0.0044516	3.5585	0.53933	1515.2	0.93161	1790.3	0.035198
15	17.575	0.0038346	0.078694	1.2388	2806.	0.97284	1037.6	0.012879
16	16.126	0.0038315	0.054164	1.3104	2813.3	0.96587	1251.4	0.011847
17	3.217	0.0044579	3.6696	0.5091	2734.6	0.96253	2187.5	0.016907
18	2.0379	0.0044775	3.0743	0.54773	3505.	0.97575	1714.	0.011701
19	0.74171	0.0043051	1.1515	0.95083	917.21	0.8782	389.93	0.018926
20	9.1316	0.0043809	5.4611	0.31327	3891.8	0.97933	6267.9	0.015196
21	7.2247	0.0043718	6.1017	0.37511	2829.2	0.95218	6376.1	0.020398
22	0.147	0.0048456	6.3485	0.41057	2164.1	0.94028	5292.6	0.050263
23	5.0611	0.0039867	2.6174	0.57957	2218.9	0.92361	6323.	0.025669
24	0.53267	0.0042968	0.39005	1.2725	1872.7	0.90776	64.166	0.030107
25	0.47697	0.0043038	0.31452	1.3289	1920.5	0.90649	45.576	0.027469
26	0.027426	0.0035443	0.031563	2.1755	1919.5	0.90099	23.902	0.025363
27	0.16383	0.0043042	0.073454	1.8592	1918.4	0.89678	27.61	0.023184
28	4.2562	0.0043737	1.5606	0.72067	1546.8	0.87958	302.02	0.040944
29	2.3508	0.0043237	2.882	0.50113	1837.7	0.89992	2377.	0.04965
30	3.1095	0.0038455	0.11477	1.5037	2184.7	0.89309	67.306	0.016588
31	15.322	0.0040306	0.65391	0.67668	3001.7	0.92484	3344.2	0.016366
32	3.6932	0.0044813	8.608	0.27638	2982.7	0.9276	3166.6	0.030874
33	7.1373	0.0043134	9.4247	0.27937	2725.8	0.91597	3166.1	0.025008
34	4.8979	0.0042937	3.7793	0.50004	2824.5	0.91028	1282.4	0.017061
35	1.3683	0.0043024	2.5679	0.60822	6907.8	0.9817	628.01	0.0068055
36	1.8301	0.0042983	2.9057	0.6038	4744.6	0.94722	936.64	0.0092242
37	0.42056	0.0041169	0.01695	2.3616	2252.7	0.89192	39.752	0.027757
38	30.78	0.0037736	0.55813	0.76816	7113.2	0.97697	1604.4	0.0065268
39	11.576	0.0042119	7.0244	0.37764	4713.5	0.94264	2493.2	0.01127
40	6.2406	0.0041916	5.2701	0.49453	4234.6	0.93232	2063.9	0.011844
41	0.33073	0.0041243	1.7246	1.1062	1930.2	0.86907	27.416	0.038208
42	0.017747	0.0041715	0.14586	1.7305	1803.6	0.86315	29.669	0.032123
43	3.7229	0.0041768	4.6286	0.56769	1678.	0.86202	3094.	0.06244
44	0.13998	0.0041329	0.25573	1.4241	1919.3	0.86326	72.797	0.032235
45	0.2859	0.0041386	0.31301	1.3424	1954.8	0.86175	115.18	0.029342
46	0.76002	0.0042179	3.386	0.76285	1867.4	0.85805	69.994	0.036448
47	6.3957	0.0041935	5.4689	0.41378	1712.6	0.85397	18493.	0.056471
48	3.4717	0.0041344	3.2337	0.63788	1116.4	0.81959	4766.	0.1179
49	2.5265	0.0042282	4.532	0.53562	1030.8	0.81652	16252.	0.19722
50	7.3683	0.0041007	4.6791	0.51428	1160.	0.82454	17965.	0.13316
51	7.7197	0.004388	3.242	0.68434	1428.1	0.83398	1786.7	0.066512
52	16.78	0.0041918	9.3198	0.29568	3370.9	0.90289	7431.7	0.02616
53	4.2132	0.0042098	4.6753	0.57945	3503.9	0.89261	1468.9	0.014359
54	4.0818	0.004214	4.4425	0.58393	3945.3	0.90281	1340.5	0.013414
55	0.18517	0.0036215	0.00058788	3.5315	2931.3	0.88936	26.18	0.026393
56	4.8248	0.0041458	6.0934	0.57026	2300.1	0.86359	2980.7	0.038679
57	0.49857	0.0041054	1.9775	0.95877	786.55	0.78509	806.6	0.40882
58	3.2754	0.0042177	5.768	0.54054	6631.3	0.94282	744.07	0.0083026
59	2.9978	0.0040901	4.5299	0.62025	2161.2	0.85669	1268.6	0.043031
60	2.8701	0.004096	4.2568	0.6138	2130.4	0.85235	1704.1	0.039385
61	10.853	0.0041149	5.8907	0.46834	2857.2	0.8755	3654.2	0.029955
62	3.6407	0.0041782	4.8742	0.57861	1267.7	0.82211	3508.2	0.24174
63	17.645	0.0040992	6.5855	0.32734	3931.3	0.90754	5156.7	0.036278
64	7.5309	0.0040814	4.9389	0.50679	2519.7	0.85819	3314.6	0.030514
65	5.4742	0.0040829	4.897	0.51113	2340.1	0.85296	2342.7	0.035662
66	4.2661	0.0040667	4.5032	0.55257	2076.4	0.84151	1666.6	0.040801
67	6.8313	0.0040486	4.3987	0.51675	2003.	0.83437	1410.4	0.03478
68	1.2707	0.0040553	4.6295	0.57428	1626.3	0.81858	995.68	0.055319
69	5.7561	0.0040491	4.357	0.52496	2207.3	0.83796	1579.5	0.027165
70	14.127	0.0040596	5.8304	0.37755	3645.9	0.87823	3411.8	0.016392
71	6.6948	0.0040603	4.9361	0.47961	2719.	0.85249	1885.8	0.019713

72	3.0619	0.0040511	3.5803	0.59082	2346.1	0.83713	1222.	0.020072
73	10.811	0.0033008	1.3767	0.76512	2003.7	0.82269	1110.6	0.024958
74	2.7101	0.0040961	1.2289	0.98598	1232.4	0.79066	155.42	0.047294
75	0.52345	0.0040244	1.4038	0.8551	1461.4	0.79677	503.34	0.036789
76	0.4616	0.0040203	1.3014	0.87043	1473.5	0.79687	443.09	0.036301
77	0.97814	0.0040374	2.0127	0.7225	1890.8	0.81747	930.7	0.02769
78	3.2086	0.004051	3.6658	0.53618	3091.2	0.85602	1508.1	0.015401
79	2.0035	0.0040431	7.4882	0.3561	4464.3	0.88836	3966.5	0.012839
80	15.43	0.0039432	1.1237	0.70703	4595.7	0.88437	1576.5	0.0088534
81	3.1512	0.0040524	4.0996	0.5425	3246.3	0.85772	1691.8	0.015058
82	7.1896	0.0040588	8.6927	0.35842	4760.6	0.88833	2888.3	0.011029
83	9.3209	0.004054	11.543	0.32027	4866.2	0.89124	3213.4	0.011935
84	29.242	0.0036195	0.16864	1.1226	5688.	0.89812	1033.3	0.0071303
85	1.8522	0.0039973	3.1556	0.65096	3755.	0.86383	1602.	0.012042
86	3.222	0.0040041	5.9024	0.52678	4040.2	0.86804	1658.4	0.011747
87	9.3412	0.0039661	7.921	0.42977	5180.9	0.88773	2173.2	0.0092007
88	36.183	0.0036003	0.58341	0.86747	6990.2	0.91082	1417.1	0.0062187
89	5.9284	0.0039695	6.4082	0.52122	4619.5	0.88083	2323.5	0.011627
90	5.2454	0.0039744	6.7969	0.48542	4586.3	0.87794	2481.5	0.011282
91	33.702	0.0036901	0.47257	0.89235	5295.7	0.8893	2053.3	0.0091908
92	2.7589	0.0039806	3.2092	0.66122	2505.4	0.82863	2065.1	0.022816

Scoef.dat continued



# File SCOEF88.asc distributed with TRIM98

Z	A	Mab	Mav	D g/cm3	D at/cm3	Vf	screen factor	subl heat		
1	001	001.0078	001.0080	00.071486	04.271	1.00000	1.00	0000	00000000000000000000	
2	004	004.0026	004.0026	00.125880	01.894	1.00000	1.00	0000	00000000000000000000	
3	007	007.0160	006.9390	00.529690	04.597	0.59782	.985	1.67	00000000000000000000	
4	009	009.0120	009.0122	01.802400	12.046	1.07810	1.06	3.38	00000000000000000000	
5	011	011.0090	010.8110	02.350200	13.093	1.04860	1.00	5.73	00000000000000000000	
.	.	.	.	.	.	.	.	.	.	.
92	238	238.0400	238.0400	19.043000	04.818	1.02570	1.16	5.42	00000000000000000000	
01	0.0121702	.00533578	1.12874	0.364197	1120.7	1.12128	2477.31	.009770990		
02	0.4890013	.0050512491	0.8613451	0.4674054	745.3815	1.0422672	7988.3889	.033328667		
03	0.8583748	.0050147482	1.6044494	0.3884424	1337.3032	1.047033	2659.2306	.018979873		
04	0.8781010	.0051049349	5.4231571	0.2031973	1200.6151	1.0211124	1401.8432	.038529280		
05	1.4607952	.0048835929	2.3380238	0.4424895	1801.2741	1.0352217	1784.1234	.020239625		
06	2.10544	.00490795	2.08723	0.46258	1779.22	1.01472	2324.45	.020269400		
07	0.645636	.00508289	4.09503	0.33879	2938.49	1.04017	2911.08	.010721900		
08	0.751093	.00503003	3.93983	0.346199	2287.85	1.01171	3997.24	.018426800		
09	1.30187	.00514136	3.82737	0.28151	2829.94	1.02762	7831.3	.020940300		
10	4.7339096	.0044505735	0.0298622	1.4940358	1825.3641	0.9789632	130.76313	.021576591		
11	6.097248	.0044291901	3.1929400	0.4576301	1363.3487	0.9518161	2380.6086	.081834623		
12	14.013106	.0043645904	2.2641223	0.3632649	2187.3659	0.9909772	6264.8005	.046200118		
13	0.0390926	.0045416623	6.9692434	0.3297639	1688.3008	0.9594386	1151.9784	.048981572		
14	2.178134	.0044454523	2.6045162	0.6088463	1550.2068	0.9330245	1703.8459	.031619771		
15	17.575478	.0038345645	0.0786935	1.2388076	2805.9699	0.9728416	1037.5875	.012878599		
Z	a	b	c	d	e	f	g	h		



# Structure of SCOEF95a

This data is used in TRIM95 and SRIM2000

At	MAI	MAI	Natural	Density	Atomic	Fermi	Heat	Proton Stopping Coefficients				Proton Stopping Coefficients.				(c) 1999 by J.F.Ziegler							
Nb	Mass	Weight	Weight	(g/cm3)	Density	Vel.	Subl	-----															
1	1	1.008	1.008	.0715	4.271E22	1.031	.00	1.28116E-02	5.33047E-03	6.51042E-01	5.31902E-01	1.95901E03	1.18870E00	5.98263E02	9.54514E-03								
2	4	4.003	4.003	.1259	1.894E22	.160	.00	3.11787E-01	4.99529E-03	1.18546E-01	9.20917E-01	9.84843E02	1.08223E00	5.54388E02	5.05072E-02								
3	7	7.016	6.941	.5340	4.633E22	.598	1.67	6.44503E-01	5.00368E-03	8.66544E-01	5.67488E-01	9.62900E02	1.01566E00	1.62034E03	2.37767E-02								
4	9	9.012	9.012	1.8480	1.235E23	1.078	3.38	9.53561E-01	5.07406E-03	1.30450E00	5.90300E-01	1.94512E03	1.05703E00	3.26951E02	1.30441E-02								
5	11	11.009	10.811	2.3502	1.309E23	1.049	5.73	1.53151E00	4.88520E-03	2.56760E00	4.23246E-01	1.73888E03	1.03208E00	1.82942E03	2.00331E-02								
6	12	12.000	12.011	2.2530	1.130E23	1.000	7.41	2.40289E00	4.91497E-03	2.49101E00	4.14939E-01	1.85836E03	1.01581E00	2.50417E03	1.81984E-02								
7	14	14.003	14.007	1.0260	4.411E22	1.058	.00	3.31007E00	4.95744E-03	5.40621E-01	7.79940E-01	1.10415E03	9.67848E-01	2.23535E03	5.31612E-02								
8	16	15.995	15.999	1.4260	5.368E22	.939	.00	9.72706E-01	5.00390E-03	1.35102E00	5.49800E-01	1.25428E03	9.68356E-01	5.09320E03	5.36453E-02								
9	19	18.998	18.998	1.1111	3.522E22	.746	.00	6.90408E-01	4.62723E-03	3.26749E-01	1.10520E00	1.30190E03	9.43525E-01	4.70373E01	2.80245E-02								
10	20	19.992	20.180	1.2040	3.593E22	.342	.00	2.81235E-01	4.59698E-03	5.25630E-01	8.78183E-01	1.15830E03	9.38564E-01	1.01606E01	4.14147E-02								
11	23	22.990	22.990	.9700	2.541E22	.453	1.12	2.15352E00	4.40847E-03	2.30923E00	6.06001E-01	1.33224E03	9.43478E-01	7.35116E02	5.77231E-02								
12	24	23.985	24.305	1.7366	4.303E22	.711	1.54	3.42983E00	4.36897E-03	2.39377E00	5.54737E-01	1.14029E03	9.29844E-01	2.10748E03	7.89342E-02								
13	27	26.982	26.982	2.7020	6.031E22	.905	3.36	3.89096E-02	4.54168E-03	4.27975E00	4.78838E-01	1.31642E03	9.34106E-01	5.65574E02	5.27220E-02								
14	28	27.977	28.086	2.3212	4.977E22	.974	4.70	1.33101E00	4.43533E-03	1.52262E00	7.75843E-01	1.22702E03	9.14146E-01	1.09117E03	4.44972E-02								
15	31	30.974	30.974	1.8219	3.542E22	.972	3.27	5.78119E00	3.98281E-03	3.24072E-01	1.22769E00	6.73459E02	8.65731E-01	1.23619E02	1.82036E-01								



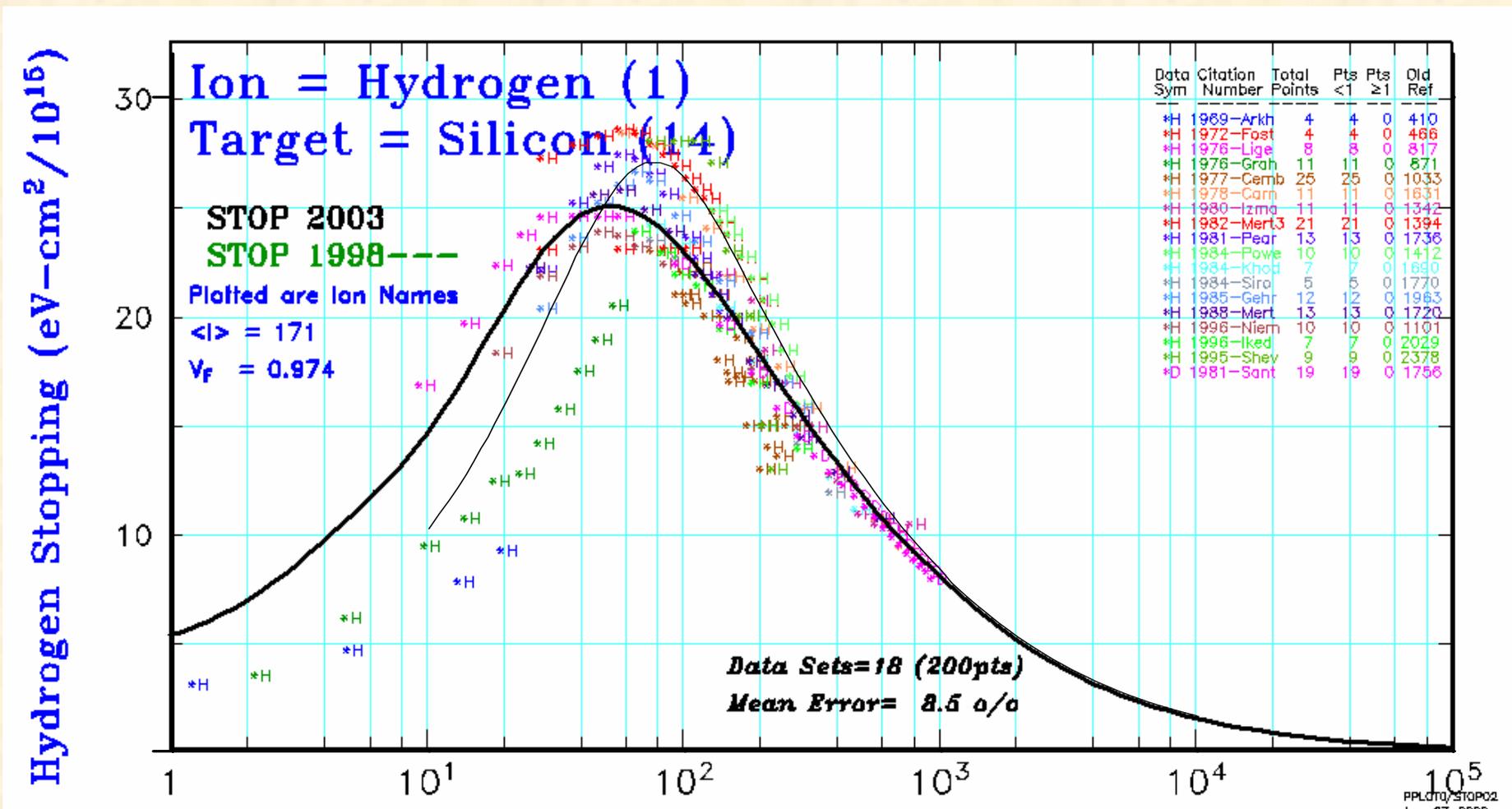
# Structure of SCOEF95b

High Energy Coefficients (>10 MeV)				Data-- Ion	Screening	Values	(Lambda)	times Z1*1/3															
				Qual	0.0	0.05	0.10	0.15	0.2	0.3	0.4	0.5	0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95	1.0	2.0	
3.95328E-03	1.91266E02	-2.74890E04	1.19093E-08	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000
7.63853E-03	3.44192E02	-4.15386E04	2.09095E-08	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000	.000
1.17654E-02	4.98615E02	-1.55328E04	2.81972E-08	9.000	.840	.810	.780	.745	.710	.640	.570	.490	.410	.400	.410	.450	.620	.830	1.150	2.000	.000	.000	.000
1.51288E-02	6.45930E02	-5.53856E04	3.79586E-08	2.000	.850	.810	.770	.730	.690	.610	.540	.460	.380	.380	.400	.480	.640	.790	.880	.850	.000	.000	.000
1.87259E-02	7.87294E02	-6.72338E04	4.61142E-08	3.000	.860	.820	.780	.750	.720	.640	.530	.420	.340	.320	.340	.460	.650	.720	.770	.620	.000	.000	.000
2.26335E-02	9.31677E02	-5.31703E04	5.32503E-08	7.000	.840	.810	.780	.735	.690	.600	.510	.430	.320	.350	.360	.440	.550	.700	.700	.400	.000	.000	.000
2.59522E-02	1.08179E03	-1.01110E05	6.34985E-08	9.000	.850	.815	.780	.720	.660	.550	.490	.400	.350	.420	.500	.520	.530	.530	.500	.310	.000	.000	.000
2.95296E-02	1.20758E03	-1.00273E05	7.00728E-08	9.000	.820	.775	.730	.700	.670	.530	.430	.330	.270	.270	.300	.350	.400	.450	.440	.250	.000	.000	.000
3.39400E-02	1.29308E03	1.96043E04	6.88358E-08	7.000	.760	.715	.670	.630	.590	.500	.420	.320	.290	.300	.370	.380	.370	.350	.340	.250	.000	.000	.000
3.59550E-02	1.44587E03	-1.55505E05	8.49021E-08	6.000	.720	.675	.630	.600	.570	.470	.330	.250	.250	.290	.330	.400	.420	.410	.340	.190	.000	.000	.000
4.05029E-02	1.55189E03	-4.56637E04	8.52664E-08	2.000	.700	.640	.580	.550	.520	.420	.340	.290	.400	.420	.420	.390	.320	.190	.110	.030	.000	.000	.000
4.29121E-02	1.70731E03	-1.88841E05	9.99305E-08	7.000	.660	.615	.570	.530	.490	.400	.320	.300	.420	.450	.420	.350	.230	.120	.000	.000	.000	.000	.000

Data	Correction to Fermi Velocity													
Qual	00	10	20	50	70	100	200	500	700	1000	2000	5000	7000	10000
.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
3.00	1.00	1.30	1.16	.98	.98	1.04	1.11	1.10	1.02	1.02	1.01	1.00	1.00	1.00
.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
9.00	1.00	1.03	.94	.88	.89	.90	.95	1.04	1.01	.97	1.01	1.00	1.00	1.00
.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00



# Comparison of SRIM2000 and SRIM2003



## Accuracy of SRIM Stopping Power Calculations

Table taken directly from [www.srim.org](http://www.srim.org)

	<b>Approx.</b>			<b>SRIM-2003</b>	<b>SRIM-2003</b>
	<b>Data Pts.</b>	<b>SRIM-1998</b>	<b>SRIM-2003</b>	<b>(within 5%)</b>	<b>(within 10%)</b>
<b>H ions</b>	<b>8300</b>	<b>4.5 %</b>	<b>4.2 %</b>	<b>74 %</b>	<b>87 %</b>
<b>He ions</b>	<b>6500</b>	<b>4.6 %</b>	<b>4.1 %</b>	<b>76 %</b>	<b>89 %</b>
<b>Li ions</b>	<b>1400</b>	<b>6.4 %</b>	<b>5.1 %</b>	<b>72 %</b>	<b>83 %</b>
<b>Be - U Ions</b>	<b>9000</b>	<b>8.1 %</b>	<b>6.1 %</b>	<b>58 %</b>	<b>82 %</b>
<b>Overall Accuracy</b>		<b>6.1 %</b>	<b>4.8 %</b>	<b>69 %</b>	<b>86 %</b>

### Table Notes:

The above table includes all data points. If wacko points are omitted (those differing from SRIM by more than 25%) then all of the above accuracy numbers would be reduced by about 20%. The overall accuracy of SRIM-2003 then reduces to 4.0%.

**Approx. Data Points** : Current total data points used in SRIM plots.

**SRIM-1998** : Comparison of SRIM-1998 stopping to experimental data. SRIM-1998 was last major change in stopping powers.

**SRIM-2003** : Current stopping power calculation

**SRIM-2003 (within 5%)** : Percentage of experimental data within 5% of the SRIM values.

**SRIM-2003 (within 10%)** : Percentage of experimental data within 10% of the SRIM values.



# Stopping in compounds

For a compound  $I_i J_j K_k \dots$  Bragg's rule of stopping power linear additivity states :

$$\mathcal{E}_{\text{compound}} = \frac{i\mathcal{E}_I + j\mathcal{E}_J + \dots}{i + j + \dots}$$

$$= \frac{\sum n\mathcal{E}_N}{\sum n}$$

e.g. 1 MeV  $^4\text{He}$  in  $\text{SiO}_2$

$$\begin{aligned}\mathcal{E}_{\text{SiO}_2} &= \frac{\mathcal{E}_{\text{Si}} + 2\mathcal{E}_{\text{O}}}{3} \\ &= \frac{61.2 + 2 \times 43.45}{3} \\ &= 49.37 \text{ eV}/10^{15} \text{ at cm}^{-2}\end{aligned}$$



# The Ziegler cores and bonds approach

For heavier elements, Bragg's rule is good, but for some lighter elements a more refined approach, based on separate additivity for atomic cores and molecular bonds gives better results. This is Ziegler's 'cores and bonds' approach.

J. F. Ziegler and J. M. Manoyan, Nucl. Inst. Methods, B35, 215-228 (1988)

```
# TABLE OF COMPOUNDS AND DATA. Table is organized as shown below.
#   The left hand character in each line indicates its purpose :
#       ! = Header for various Tables      (e.g. Nuclear Materials, Gases...)
#       * = Target Description for Table   (e.g. Air, Bone, Water...)
#   Next Line = Numerical Data-Line for target. Data Line is :
#       (Name), (Density g/cm3), (Number of elements), (Atomic No.), (Atom %), ...
#       !!!! Maximum Number of elements in a target = 8,
#   NOTE: Can use composition by Mass Percent (Indicate by preceding Name by "%")
#       For example, for BONE in both Atomic percent and Mass percent:
#       Atomic % = "Bone" ,1.92,6, 1,39.3, 6,15.1, 7,3.5, 8,31.7, 40,6.5, 15,3.9
#       Mass    % = "%Bone",1.92,6, 1,3.37, 6,1.29, 7,0.3, 8,2.72, 40,0.56,15,0.33
#   Next Line = Numerical Bond-Structure data for target. Bonding Line is :
#       (H-H) (H-C) (H-N) (H-O) (C-C) (C=C) (C≡C) (C-N) (C-O) (C=O) (C-F) (C-Cl)
#       (N≡N) (N-O) (O=O) (S-H) (S-C) (S-F)
#       $ = Comments on target (maximum of 8 lines / target)
#   ***   After the above is input, the next compound starts.
#   ***   Look at some of the examples below, and this will be clearer.
#-----
```



# Compound.dat entries : water

```
!
! ██████████ NUCLEAR PHYSICS MATERIALS ██████████
!
!           Density           Atomic Stoichiometry
! Common Name           (g/cm3)           (Atoms/Molecule or Atom Percent)
!=====
*Air           .00125           O-23.2, N-75.5, Ar-1.3
"Air", .00125, 3, 8, 23.2, 7, 75.5, 18, 1.3
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
$
*Water (liquid)           1.00           H-2, O-1
"Water_Liquid", 1.0, 2, 1, 2, 8, 1
0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
$Chemical Formula:      H — O — H
$
$There is about an 8% increase in the peak of the stopping power
$for ions in water vapour relative to the liquid. (The peak of the
$stopping occurs at an energy of about 100 keV/amu times the 2/3
$power of the ion's atomic number.) Above the peak the phase
$difference begins to disappear. This calculation is for the
$LIQUID phase.
*Water (vapor)           (gas)           H-2, O-1
"Water_vapor", 0.00125, 2, 1, 2, 8, 1
0 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
$Chemical Formula:      H — O — H
$
$There is about an 8% increase in the peak of the stopping power
$for ions in water vapour relative to the liquid. (The peak of the
$stopping occurs at an energy of about 100 keV/amu times the 2/3
$power of the ion's atomic number.) Above the peak the phase
$difference begins to disappear. This calculation is for the
$GAS phase.
```



# Compound.dat entries : concrete, graphite, paraffin

```

*Concrete                2.34 (±.15)    C-23,O-40,Si-12,Ca-12,H-10,Mg-2
"Concrete", 2.34, 6, 6, 23, 8, 40, 14, 12, 20, 12, 1, 10, 12, 2
0 0 0 0  0 0 0 0 0 0 0 0  0 0 0  0 0 0
$Concrete has a wide variation in density and composition. The above
$description is for poured structural concrete with 10% moisture
$content. Concrete block will have a density of about 2.05 g/cm3.
$Ranges of concrete composition are : C (8-25%), O (38-60%), Si (8-18%).
$Concrete composition can be analyzed cheaply by commercial laboratories.
$
*Graphite (carbon)      2.26            C-6
"Graphite (carbon)", 2.26, 1, 6, 6
0 0 0 0  6 3 0 0 0 0 0 0  0 0 0  0 0 0
$Chemical      — C = C —
$Formula      /       \
$             — C     C —
$             \\      //
$             — C — C —
$Graphite has a wide variation in density and composition. There are
$several different layered structures called graphite. The above
$formulation is typical.
*Paraffin            0.89            H-2, C-1
"Paraffin", 0.89, 2, 1, 2, 6, 1
0 2 0 0  1 0 0 0 0 0 0 0  0 0 0  0 0 0
$Density variation of paraffin is 0.87 - 0.91 g/cm3.
$Chemical      H     H
$Formula      |     |
$             — C — C —
$             |     |
$             H     H

```



# ICRU Report 49

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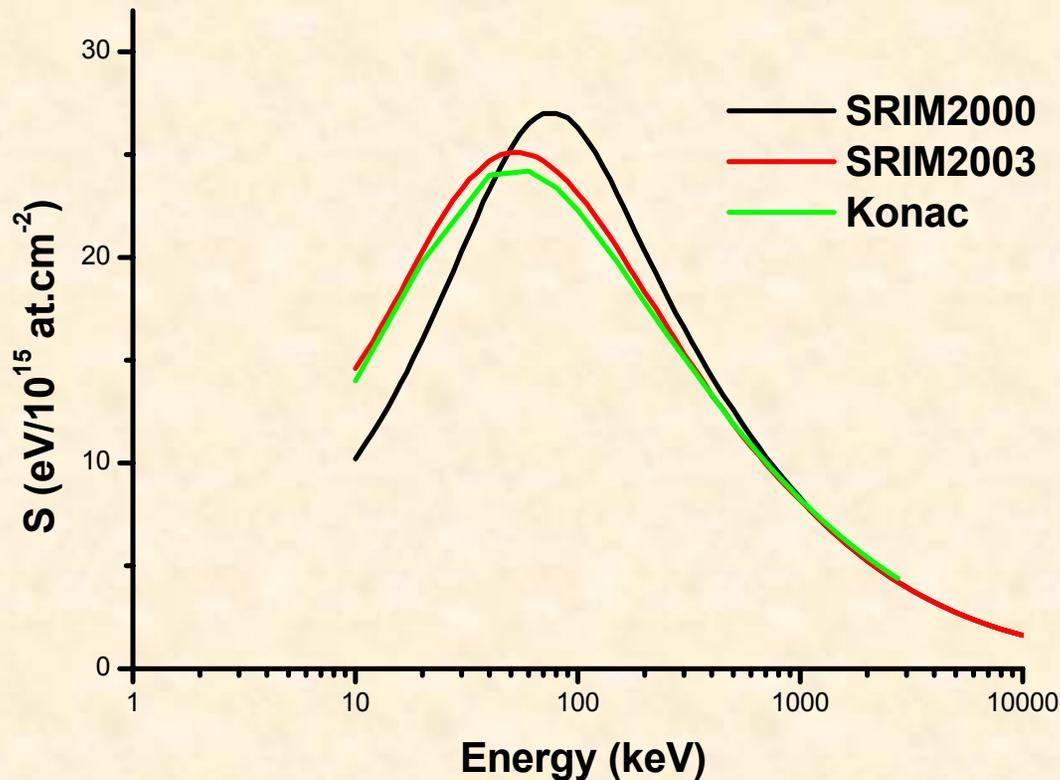
Published in 1992/3 - refers primarily to pre-1985 Ziegler, Biersack, Varelas formulations and semi-empirical fits.

Has a good general presentation of the main elements of stopping theory for light rapid particles, and fairly comprehensive description of different measurement methods.



# Konac et al stopping powers

## Protons in Silicon



$$S_e(E) = \frac{E^s \ln(e + \beta E)}{P(E)}$$

$$P(E) = \alpha_0 + \alpha_1 E^{1/4} + \alpha_2 E^{1/2} + \alpha_3 E^{1+s}$$

G. Konac et al. NIMB 136-138 (1998) 159-165  
H and He in Si, C 1-1000 keV/amu

maximum difference ~1% for  
protons in Si

$$S_e(E) = \frac{E^s \ln(e + \beta E)}{P(E)}$$

$$P(E) = \alpha_0 + \alpha_1 E^{1/2} + \alpha_2 E + \alpha_3 E^{1+s}$$

G. Konac et al. NIMB 146 (1998) 159-165  
All ions in C and Si 0.01-100 MeV/amu



Table 1  
Fit parameters for  $S(E)$  and  $W(E)$  curves <sup>a</sup>

	<sup>1</sup> H/Si	<sup>2</sup> H/Si	<sup>1</sup> H/C	<sup>3</sup> He/Si	<sup>4</sup> He/Si	<sup>4</sup> He/C
$s^b$	0.37	0.37	0.39	0.52	0.52	0.49
$\alpha_0$	$4.16 \times 10^{-2}$	$3.66 \times 10^{-2}$	$3.40 \times 10^{-2}$	$8.24 \times 10^{-3}$	$7.93 \times 10^{-3}$	$1.36 \times 10^{-3}$
$\alpha_1$	$-1.47 \times 10^{-1}$	$-1.24 \times 10^{-1}$	$-3.93 \times 10^{-2}$	$-2.02 \times 10^{-2}$	$-1.93 \times 10^{-2}$	$2.47 \times 10^{-2}$
$\alpha_2$	$1.80 \times 10^{-1}$	$1.52 \times 10^{-1}$	$2.09 \times 10^{-2}$	$2.28 \times 10^{-2}$	$2.21 \times 10^{-2}$	$-1.81 \times 10^{-2}$
$\alpha_3^c$	$2.79 \times 10^{-1}$	$2.93 \times 10^{-1}$	$7.89 \times 10^{-1}$	$8.18 \times 10^{-2}$	$8.25 \times 10^{-2}$	$1.88 \times 10^{-1}$
$\beta^d$	15.7	15.7	36.5	15.7	15.7	36.5
$bM_1^e$	17.2	16.2	14.9	10.5	10.0	6.4

<sup>a</sup> Use reduced energies  $E/M$  in units of MeV/amu in Eqs. (1) and (2) for  $E$  to obtain  $S_e(E)$  in units of  $\text{eV cm}^2/10^{15}$  at and  $W_e(E)$  in units of  $\text{eV}^2 \text{cm}^2/10^{12}$  at. Fitted range:  $1 \leq E/M \leq 1000$  keV/amu.

<sup>b</sup> For Si the exponents  $s$  were derived by comparing backscattering spectra for H and He isotopes [21], whereas those for C are best fit values as obtained by use of Eq. (1).

<sup>c</sup> Bethe/Bloch theory:  $\alpha_3 E = kE/8\pi Z_1^2 Z_2 e^4$ ,  $k = 4m/M$ ; these values differ by about 10% from those listed.

<sup>d</sup> Figures obtained by use of the Bethe/Bloch relation:  $\beta E = kE/I_0 Z_2$ ,  $k = 4m/M$ , with  $I_0 = 10$  eV.

<sup>e</sup>  $bM$  is given in units of (amu/MeV).

G. Konac et al. NIMB 136-138 (1998) 159-165  
H and He in Si, C 1-1000 keV/amu

# Konac coefficients

G. Konac et al. NIMB 146 (1998) 159-165  
All ions in C and Si 0.01-100 MeV/amu

Table 2  
Fit coefficients for electronic stopping cross-sections in silicon. Energy range:  $0.01 \leq E \leq 100$  MeV/amu

Ion	$s$	$\alpha_0$	$\alpha_1$	$\alpha_2$	$\alpha_3$	$\beta^a$
<sup>1</sup> H	0.68	$3.64 \times 10^{-3}$	$-9.70 \times 10^{-3}$	$5.90 \times 10^{-2}$	$3.12 \times 10^{-1}$	15.7
<sup>4</sup> He	0.63	$2.73 \times 10^{-3}$	$-4.95 \times 10^{-3}$	$2.32 \times 10^{-2}$	$7.03 \times 10^{-2}$	15.7
<sup>13</sup> C	0.53	$1.30 \times 10^{-3}$	$-6.12 \times 10^{-4}$	$6.55 \times 10^{-3}$	$6.89 \times 10^{-3}$	15.7
<sup>48</sup> Ti	0.52	$7.94 \times 10^{-4}$	$-9.74 \times 10^{-5}$	$1.19 \times 10^{-3}$	$4.33 \times 10^{-4}$	15.7
<sup>52</sup> Cr	0.53	$7.13 \times 10^{-4}$	$-6.35 \times 10^{-5}$	$1.17 \times 10^{-3}$	$3.28 \times 10^{-4}$	15.7
<sup>58</sup> Ni	0.55	$6.91 \times 10^{-4}$	$-6.63 \times 10^{-5}$	$9.34 \times 10^{-4}$	$2.58 \times 10^{-4}$	15.7
<sup>74</sup> Ge	0.51	$7.51 \times 10^{-4}$	$-4.15 \times 10^{-5}$	$7.41 \times 10^{-4}$	$1.86 \times 10^{-4}$	15.7
<sup>79</sup> Br	0.52	$6.26 \times 10^{-4}$	$-4.25 \times 10^{-5}$	$7.06 \times 10^{-4}$	$1.45 \times 10^{-4}$	15.7
<sup>93</sup> Nb	0.53	$5.49 \times 10^{-4}$	$-2.82 \times 10^{-5}$	$6.02 \times 10^{-4}$	$1.02 \times 10^{-4}$	15.7
<sup>107</sup> Ag	0.49	$6.15 \times 10^{-4}$	$-1.74 \times 10^{-5}$	$4.45 \times 10^{-4}$	$7.58 \times 10^{-5}$	15.7
<sup>127</sup> I	0.51	$5.48 \times 10^{-4}$	$-1.85 \times 10^{-5}$	$4.03 \times 10^{-4}$	$6.02 \times 10^{-5}$	15.7
<sup>197</sup> Au	0.51	$4.55 \times 10^{-4}$	$-9.20 \times 10^{-6}$	$2.65 \times 10^{-4}$	$2.15 \times 10^{-5}$	15.7
<sup>209</sup> Bi	0.51	$4.49 \times 10^{-4}$	$-8.70 \times 10^{-6}$	$2.53 \times 10^{-4}$	$1.85 \times 10^{-5}$	15.7

<sup>a</sup> Obtained by use of the Bethe-Bloch formula with a mean ionization potential of  $I = Z_2 \times I_0 = 140$  eV [6].



# Special case of 2 MeV $^4\text{He}$ in Si

Climent-Font, A., U. Watjen, et al. (1992). *Quantitative RBS Analysis using RUMP. On the accuracy of the He stopping in Si.* Nuclear Instruments & Methods in Physics Research, Section B (Beam Interactions with Materials and Atoms) **71**: 81-86.

- "Rump" stopping is 10% or so too high (TRIM85 or 98 stopping powers).

W.N. Lennard, G.R. Massoumi, T.W. Simpson, I.V. Mitchell, Nucl. Instr. and Meth. B 152 (1999) 370.

- Konac et al measurement confirmed

M. Bianconi, F. Abel, J.C. Banks, A. Climent Font, C. Cohen, B.L. Doyle, R. Lotti, G. Lulli, R. Nipoti, I. Vickridge, D. Walsh, E. Wendler. *The Si surface yield as a calibration standard for RBS.* Nuclear Instruments and Methods in Physics Research B 161-163 (2000) 293-296.

- RBS surface plateau height for  $^4\text{He}$ , 1-3 MeV, good with Konac stopping powers

N.P. Barradas, C. Jeynes, R.P. Webb, E. Wendler. *Accurate determination of the stopping power of  $^4\text{He}$  in Si using Bayesian Inference.* Nucl. Instr. And Meth. B 194 (2002) 15-25.

2% correction to above three papers

	a	b	c	d	e	f	g	h
ZBL	2.072	0.0044516	3.5585	0.53933	1515.3	0.93161	1790.3	0.035198
Barradas	0.6286	0.0422970	3.3416	0.54056	1499.7	0.93180	2042.1	0.033552



# Bianconi values

Amorphised Si target, interlaboratory comparison to determine plateau heights  $H_0$

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*M. Bianconi et al. / Nucl. Instr. and Meth. in Phys. Res. B 161-163 (2000) 293-296*

Table 3

Surface RBS yield ( $H_0$ ) for Si as a function of the energy calculated using different stopping power data available in the literature (see text)<sup>a</sup>

	$H_0$ counts/( $\mu\text{C msr keV}$ )				
	1.0 MeV	1.5 MeV	2.0 MeV	2.5 MeV	3.0 MeV
Experiment	58.5	28.8	18.3	12.7	9.47
RUMP	57.2	27.7	17.1	12.0	9.06
SRIM2000	57.6	28.1	17.3	12.1	9.09
KKKNS	60.5	29.5	18.3	12.8	9.69

<sup>a</sup>The average experimental data are shown for comparison.



## Particular case : 150 keV protons in SiO<sub>2</sub>

Nuclear resonance profiling via  $^{18}\text{O}(\text{p},\alpha)^{15}\text{N}$

A value of 475 keV/mg.cm<sup>-2</sup> has been largely verified by comparison with multiple complementary methods in Paris.

SRIM 2000 value : 509 keV/mg.cm<sup>-2</sup>

SRIM 2003 value : 502 keV/mg.cm<sup>-2</sup>

**Conclusion** : The semi-empirical fits from SRIM undoubtedly provide the best overall summary of our knowledge of stopping powers, however in any particular case they may vary by more than 10% from the 'true' value that only God knows.

*If you have a solid and reliable measurement, use that rather than the SRIM value.*



# What we haven't talked about

## Phase effects

Much stopping data (e.g. N<sub>2</sub>, O<sub>2</sub>) has been measured in gas targets. The stopping power of these atoms in solids is not necessarily the same as in the gas phase. This also the case for inert gases, however here there is no phase effect (J. Ziegler, pers.comm.) (Van der Waals solids)

## Heavy ion stopping

A similar  $Z^2$  scaling rule from proton stopping is applied. All the hard work is concerned with finding the effective charge of the ion in the stopping medium



# Exercices

**1. *Getting stopping power values.***

Compare the values of stopping for 2 MeV  $^4\text{He}$  in silicon from TRIM98, SRIM2000, SRIM2003, and the values found by Konacs et al, Lennard et al, and Bianconi et al. Compare these values with that determined from the 1985 TRIM book.

**2. *Compare calculation with data***

Compare the calculated SRIM2003 value with data, via the website [www.srim.org](http://www.srim.org). You can also browse other entries, including tutorials and physics on this extensive site

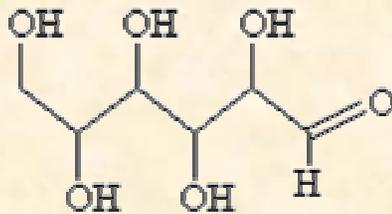
**3. *Build a TRIM entry for a new compound* :e.g. sucrose using cores and bonds approach**

**4. *Investigate phase effects.*** E.g. try SRIM for water vapour and liquid water.



# Glucose data

Example : glucose  $C_6H_7(OH)_5O$ ,  $\rho=1.5 \text{ g.cm}^{-3}$



The Chain form of Glucose



The Ring form of Glucose

