The Abdus Salam
International Centre for Theoretical Physics

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Joint ICTP/IAEA Workshop on Advanced Simulation and Modelling for Ion Beam Analysis

23 - 27 February 2009

IBA Intro VI Energy Loss, SRIM, etc

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Joint ICTP/IAEA Workshop on Advanced Simulation and Modelling for Ion Beam Analysis, 23-27 February 2009

IBA Intro VI

Energy Loss, SRIM, etc

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Instituto Tecnológico e Nuclear

Overview

- Introduction
- Energy loss of ions in matter
- SRIM today – statistical analyis
- Conclusions

Introduction

2

THE

LONDON, EDINBURGH, AND DUBLIN

PHILOSOPHICAL MAGAZINE

AND

JOURNAL OF SCIENCE.

[SIXTH SERIES.]

APRIL 1912.

XLII. *Ionization by Moving Electrified Particles.* *By* Sir J. J. THOMSON*.

THE theory developed in this paper is based on the following assumptions:—

1. Cathode or positive rays when they pass through an atom repel or attract the corpuscles in it and thereby give to them kinetic energy.
2. When the energy imparted to a corpuscle is greater than a certain definite value—the value required to ionize the atom—a corpuscle escapes from the atom, and a free corpuscle and positively charged atom are produced.

We must first find under what circumstances a cathode ray moving with a given velocity will lose when it passes by a corpuscle a quantity of energy greater than the amount required to ionize an atom.

In my 'Conduction of Electricity through Gases' it is shown that when a body with a charge E_1 in electrostatic units and mass M_1 is projected with a velocity V towards a body with a charge E_2 and mass M_2 at rest, the energy Q transferred to the latter is given by the equation

$$Q = \frac{4M_1M_2}{(M_1+M_2)^2} T \sin^2\theta,$$

* Communicated by the Author.

Phil. Mag. S. 6. Vol. 23. No. 136. *April* 1912. 2 H

Figure (1-1) A reproduction of the first extended theoretical paper on the energy loss of charged particles in matter.

THE

LONDON, EDINBURGH, AND DUBLIN

PHILOSOPHICAL MAGAZINE

AND

JOURNAL OF SCIENCE.

[SIXTH SERIES.]

JANUARY 1913.

II. *On the Theory of the Decrease of Velocity of Moving Electrified Particles on passing through Matter.* *By* N. BOHR, *Dr. phil. Copenhagen**.

WHEN cathode-rays or α- and β-rays penetrate through matter their velocity decreases. A theory of this phenomena was first given by Sir J. J. Thomson†. In the calculation of this author the cathode- and β-rays are assumed to lose their velocity by collisions with the electrons contained in the atoms of the matter. The form of the law, found by this calculation, connecting the velocity of the particles and the thickness of matter traversed, has been recently shown by Whiddington‡ to be in good agreement with experiments. Somewhat different conceptions are used in the calculation of Sir J. J. Thomson on the absorption of α-rays, as the latter, on account of their supposed greater dimensions, are assumed to lose their velocity by collisions, not with the single electrons but with the atoms of the matter considered as entities.

According to the theory given by Professor Rutherford§ of the scattering of α-rays by matter, the atoms of the matter are supposed to consist of a cluster of electrons kept together by attractive forces from a nucleus. This nucleus, which possesses a positive charge equal to the sum of the negative charges on the electrons, is further supposed to be the seat of the essential part of the mass of the atom, and to have dimensions which are exceedingly small compared with the dimensions of the atom. According to this theory an α-particle consists simply of the nucleus of a helium atom. We see that after such a conception there is no reason to discriminate materially between the collisions of an atom with an α- or β-particle—apart of course from the differences due to the difference in their charge and mass.

An elaborate theory of the absorption and scattering of α-rays, based on Professor Rutherford's conception of the constitution of atoms, was recently published by C. G. Darwin‖. In the theory of this author the α-particles simply penetrate the atoms and act upon the single electrons contained in them, by forces varying inversely as the square

* Communicated by Prof. E. Rutherford, F.R.S.
† J. J. Thomson, 'Conduction of Electricity through Gases,' pp. 370–382.
‡ R. Whiddington, Proc. Roy. Soc. A. lxxxvi. p. 360 (1912).
§ E. Rutherford, Phil. Mag. xxi. p. 669 (1911).
‖ C. G. Darwin, Phil. Mag. xxiii. p. 907 (1912).

THE

LONDON, EDINBURGH, AND DUBLIN

PHILOSOPHICAL MAGAZINE

AND

JOURNAL OF SCIENCE.

[SIXTH SERIES.]

OCTOBER 1915.

LX. *On the Decrease of Velocity of Swiftly Moving Electrified Particles in passing through Matter.* *By* N. BOHR, *Dr. Phil. Copenhagen; p. t. Reader in Mathematical Physics, University of Manchester**.

THE object of the present paper is to continue some calculations on the decrease of velocity of α and β rays published by the writer in a previous paper in this magazine†. This paper was concerned only with the mean value of the rate of decrease of velocity of the swiftly moving particles, but from a closer comparison with the measurements it appears necessary, especially for β rays, to consider the probability distribution of the loss of velocity suffered by the single particles. This problem has been discussed briefly by K. Herzfeld‡, but on assumptions as to the mechanism of decrease of velocity essentially different from those used in the following*. Another question which will be considered more fully in the present paper is the effect of the velocity of β rays being comparable with the velocity of light. These calculations are contained in the first three sections. In the two next sections the theory is compared with the measurements. It will be shown that the approximate agreement obtained in the former paper is improved by the closer theoretical discussion, as well as by using the recent more accurate measurements. Section 6 contains some considerations on the ionization produced by α and β rays. A theory for this phenomenon has been given by Sir J. J. Thomson†.

§ 1. *The average value of the rate of decrease of velocity.*

For the sake of clearness it is desirable to give a brief summary of the calculations in the former paper. References to the previous literature on the subject will be found in that paper.

Following Sir Ernest Rutherford, we shall assume that the atom consists of a central nucleus carrying a positive charge and surrounded by a cluster of electrons kept together by the attractive forces from the nucleus. The nucleus is the seat of practically the entire mass of the atom and has dimensions exceedingly small compared with the dimensions of the surrounding cluster of electrons. If an α or β particle passes through a sheet of matter it will penetrate

Figure (1-2) Reproductions of the first two papers by Neils Bohr on the stopping of charged particles in matter. Bohr had finished his Ph.D. in 1911. After an unsympathetic visit with J. J. Thomson, Bohr went to work with Rutherford at the Manchester Laboratory and produced these papers. Between these papers he also developed and published his theory of the atom which suggested the quantization of angular momentum.

Introduction

THE

PHYSICAL REVIEW

A Journal of Experimental and Theoretical Physics Established by E. L. Nichols in 1893

MARCH 15, 1940 PHYSICAL REVIEW VOLUME 57

The Ionization Loss of Energy in Gases and in Condensed Materials*

ENRICO FERMI
Pupin Physics Laboratories, Columbia University, New York, New York

(Received January 22, 1940)

It is shown that the loss of energy of a fast charged particle due to the ionization of the material through which it is passing is considerably affected by the density of the material. The effect is due to the alteration of the electric field of the passing particle by the electric polarization of the medium. A theory based on classical electrodynamics shows that by equal mass of material traversed, the loss is larger in a rarefied substance than in a condensed one. The application of these results to cosmic radiation problems is discussed especially in view of the possible explanation on this basis of part of the difference in the absorption of mesotrons in air and in condensed materials that is usually interpreted as evidence for a spontaneous decay of the mesotron.

THE determination of the energy lost by a fast charged particle by ionization and excitation of the atoms through or near which it is passing has been the object of several theoretical investigations. The essential features of the phenomenon are explained as well known

* Publication assisted by the Ernest Kempton Adams Fund for Physical Research of Columbia University.

OCTOBER 1, 1940 PHYSICAL REVIEW VOLUME 58

Scattering and Stopping of Fission Fragments

N. BOHR
Institute of Theoretical Physics, University of Copenhagen, Copenhagen, Denmark

(Received July 9, 1940)

THE cloud-chamber pictures of tracks of uranium fission fragments in gases obtained by Brostrøm, Bøggild and Lauritsen[1] have revealed a number of interesting differences between such tracks and those of protons and alpha-particles. These differences may be simply shown to be caused by the comparatively high charge and mass of the fission fragments, which imply that nuclear collisions play a much greater part in the phenomenon than is the case for the ordinary light particles.

will have orbital velocities greater than or equal to V.

In an encounter between the fragment and a heavy atom possessing electrons lightly bound and also electrons with velocities greater than V, we may, moreover, assume that only the former electrons, in approximate number V/V_0, will be effective in the stopping. This is true since the faster electrons, just as the electrons carried with the fragment, will be merely adiabatically influenced during the encounter and will therefore

Figure (1-4) Reproductions of the articles in The Physical Review in 1940-1941 which shows that interest had now shifted to the stopping of heavy fission fragments and the development of heavy ion stopping-power scaling theory.

MATHEMATISK-FYSISKE

MEDDELELSER

DET KGL. DANSKE VIDENSKABERNES SELSKAB

THE PENETRATION OF ATOMIC PARTICLES THROUGH MATTER

BY

NIELS BOHR

Mathematisk-fysiske Meddelelser **XVIII**, 8.

ON THE PROPERTIES OF A GAS OF CHARGED PARTICLES

BY

J. LINDHARD

Dan. Mat. Fys. Medd. **28**, no. 8 (1954)

RANGE CONCEPTS AND HEAVY ION RANGES

(NOTES ON ATOMIC COLLISIONS, II)

BY

J. LINDHARD, M. SCHARFF(†) AND H. E. SCHIØTT

Mat. Fys. Medd. Dan. Vid. Selsk. **33**, no. 14 (1963)

Figure (1-6) Reproductions of the articles in the Danish journal of mathematical physics. After World War II, Niels Bohr settled in Copenhagen and created a broad interest in the theory of the stopping and range of ions in matter; of special note are the many papers by his student, Jens Lindhard, and his collaborators.

Introduction

1900 Marie Curie: “les rayons alpha sont des projectiles materiels susceptibles de perdre de leur vitesse en traversant la matiere”.

1913 Bohr: Unified analysis of stopping of charged particles in matter. Nuclear and electronic stopping.

1930s Bethe and Bloch: Stopping of fast particles in a quantised electron plasma.

1940s Stopping of fission fragments - partially stripped heavy ions, Thomas-Fermi atom. Scaling to H stopping values.

1954 Lindhard: full non-relativistic treatment of particle interactions with a free-electron gas.

1963 Lindhard, Scharff Schiott (LSS): Unified approach to stopping and range, over the entire range of atomic species

1960s Numerical methods, Hartree-Fock atoms.

1980-2009 Ziegler, Biersack, Littmark (ZBL): Vast amounts of experimental data integrated in semi-empirical data-base. Ion implantation, Ion beam analysis.

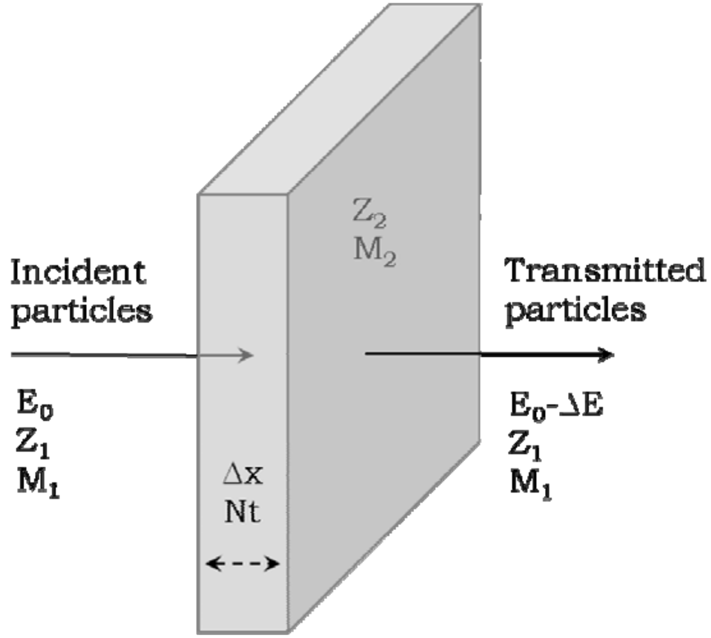
Energy loss of ions in matter

Basic concepts

Energy loss dE/dx $\lim_{\Delta x \to 0} \Delta E / \Delta x \equiv \frac{dE}{dx}(E)$

often called stopping power

units e.g. MeV/mm, eV/μm



Stopping cross section ε

$\varepsilon = (1/N)(dE/dx)$ or $\varepsilon = (1/\rho)(dE/dx)$

N: volume density ρ : mass density

units e.g. eV/10^{15} at/cm^2

$$E(x) = E_0 - \int_0^x (dE/dx) \quad dx$$

$$x = \int_E^{E_0} (dE/dx)^{-1} \quad dE$$

Elemental targets vs. mixtures and compounds

- Bragg rule very often used

$$\varepsilon^{AB} = m\varepsilon^{A} + n\varepsilon^{B}$$

- Pretty good for metallic compounds
- Deviations can be around 10-20% for oxides, nitrides, etc
- Measured molecular stopping power may have to be used

Stopping powers – printed compilations

Whaling (1958)
Northcliffe and Schilling (1970)
Johnson and Gibbons (1970)
Bichsel (1972)
Brice (1975)
Ziegler and Chu (1974)
Gibbons et al. (1975)
Winterbon (1975)
Andersen and Ziegler (1977)
Hubert et al. (1980)

Littmark and Ziegler (1980)
Ziegler (1977, 1980)
Janni (1982)
Ziegler et al. (1985)
Hubert et al. (1990)
Berger and Paul (1995)
ICRU report 49 (1993)
Paul and Schinner (2003)
Ziegler (2004)
ICRU report 73 (2005)

Stopping powers – web compilations

SRIM (J.F. Ziegler):
http://www.srim.org/
Stopping Power for Light Ions (H. Paul):
http://www.exphys.uni-linz.ac.at/stopping/

Stopping powers – computer programs

ASTAR and **PSTAR** (M.J. Berger, J.S. Coursey, M.A. Zucker, J. Chang):
http://www.exphys.uni-linz.ac.at/stopping/
ATIMA (H. Geissel, C. Scheidenberger, P. Malzacher, J. Kunzendorf, H. Weick):
http://www-linux.gsi.de/~weick/atima/
CASP (P.L. Grande and G. Schiwietz):
http://www.hmi.de/people/schiwietz/casp.html
GEANT4 (Geant4 collaboration):
http://geant4.web.cern.ch/geant4/
MSTAR (H.Paul and A.Schinner):
http://www.exphys.uni-linz.ac.at/stopping/
SRIM (J.F. Ziegler):
http://www.srim.org/

Energy loss of ions in matter

Nuclear and electronic stopping

$$\varepsilon = \varepsilon_n + \varepsilon_e$$

ignores correlations, which are averaged over many collisions

v: ion velocity $v_0 = e^2/\hbar$: Bohr velocity electron in innermost orbit of H atom

Nuclear stopping ε_n From many small-angle scattering collisions of projectile with nuclei of target. Elastic interaction between two free particles (down to ~ 10 eV of chemical binding).

Dominates at v<<vo. The projectile is neutralised and carries its electrons. Electric interaction is minimised and elastic collisions with the target nuclei dominate the energy loss.

Energy loss of ions in matter

Calculation of nuclear stopping

Interaction potential $V = V_{nn} + V_{en} + V_{ee} + V_k + V_a$

Vnn: electrostatic interaction between the two nuclei
Vee: pure electrostatic interaction between the electron distributions
Ven: between nucleus and electron distribution
Vk: increase in kinetic energy of electrons in overlap region due to Pauli excitation
Va: increase in exchange energy of electrons in overlap region

$V_c = V_{nn} + V_{en} + V_{ee}$:Coulombic contribution

We shall omit quantum-mechanical effects and polarisation

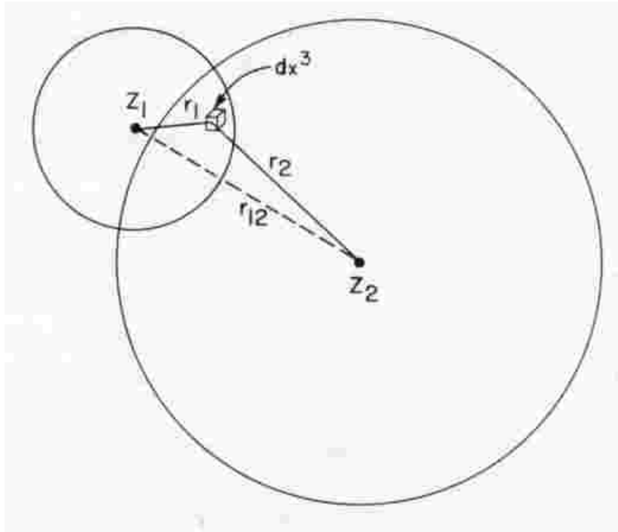
Energy loss of ions in matter

Calculation of nuclear stopping

$$V_{nn} = Z_1 Z_2 e^2 / r_{12}$$

$$V_{en} = -Z_1 e^2 \left[\Psi_2(r_{12}) + Q_2(r_{12})/ r_{12}\right]$$

$$V_{ee} = e^2 \int \left[\Psi_2(r_2) + Q_2(r_2)/ r_2\right]\rho_1 \, d x^3$$



Totally degenerate free electron gas: change in kinetic energy in the region of electronic overlap:

$$V_a = -\left[\frac{3e^2}{4}\left(\frac{3}{\pi}\right)^{1/3}\right]\int\left[(\rho_1+\rho_2)^{4/3} - \left(\rho_1^{\,4/3} + \rho_2^{\,4/3}\right)\right] d x^3$$

Pauli principle: partial electron depletion in vicinity of each electron. Lower local electron density lowers energy of the system:

$$V_k = \left[\frac{3}{5}\frac{\hbar^2 \pi^2}{2m}\left(\frac{3}{\pi}\right)^{2/3}\right]\int\left[(\rho_1+\rho_2)^{5/3} - \left(\rho_1^{\,5/3} + \rho_2^{\,5/3}\right)\right] d x^3$$

Energy loss of ions in matter

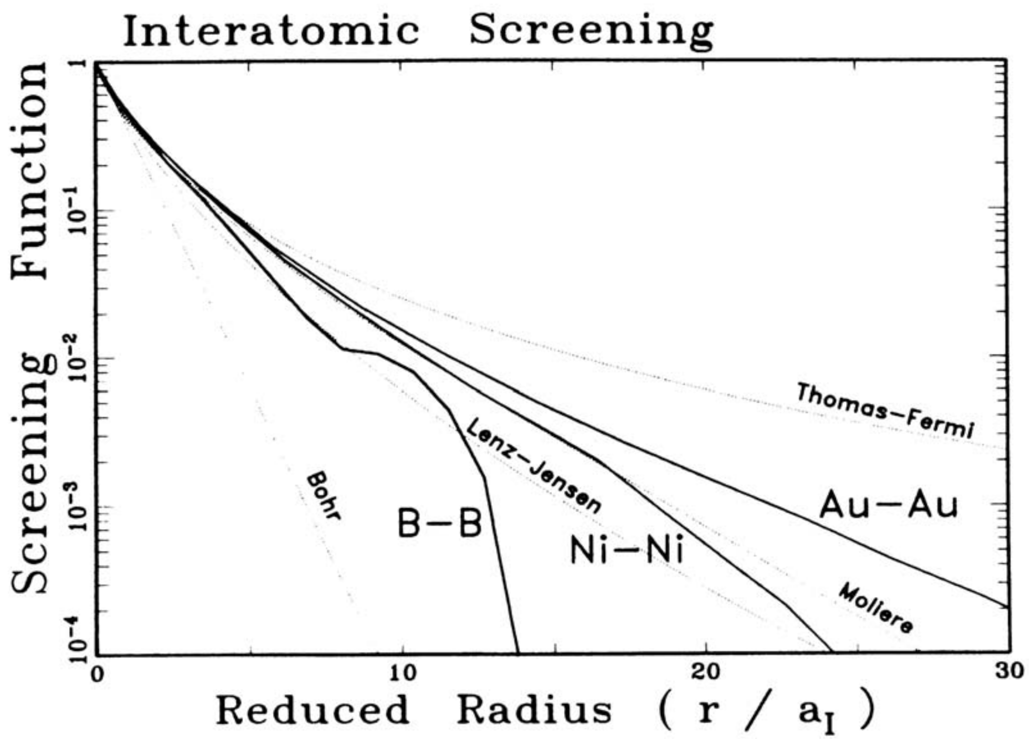
Calculation of nuclear stopping

Interatomic screening function

$$\Phi_I = \frac{V(r)}{Z_1 Z_2 e^2 / r}$$

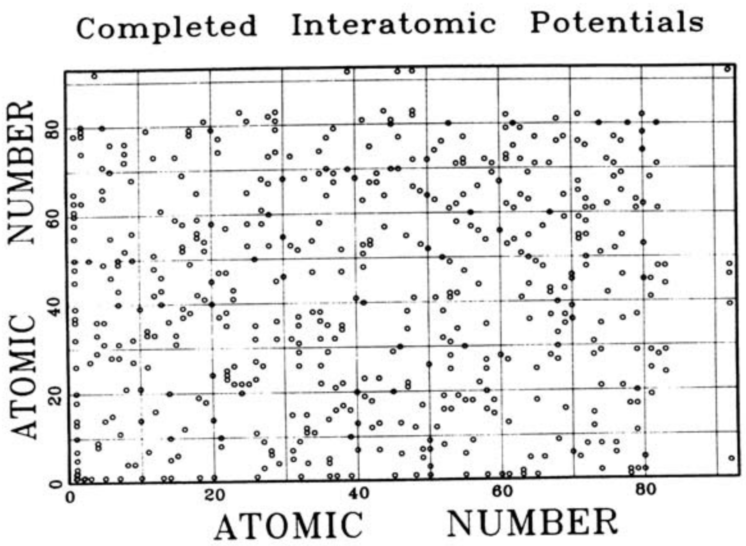
Reduced radius (Linhard)

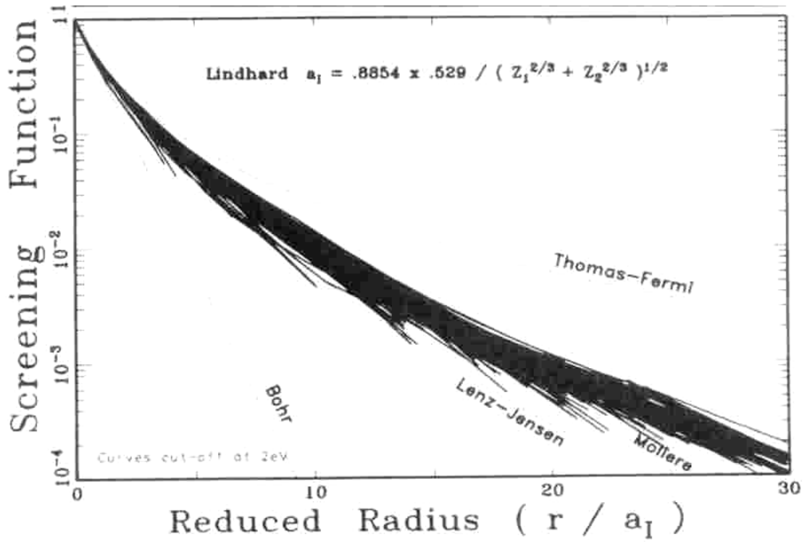
$$a_I = \frac{0.8853\, a_0}{\left(Z_1^{2/3} + Z_2^{2/3}\right)^{1/2}}$$

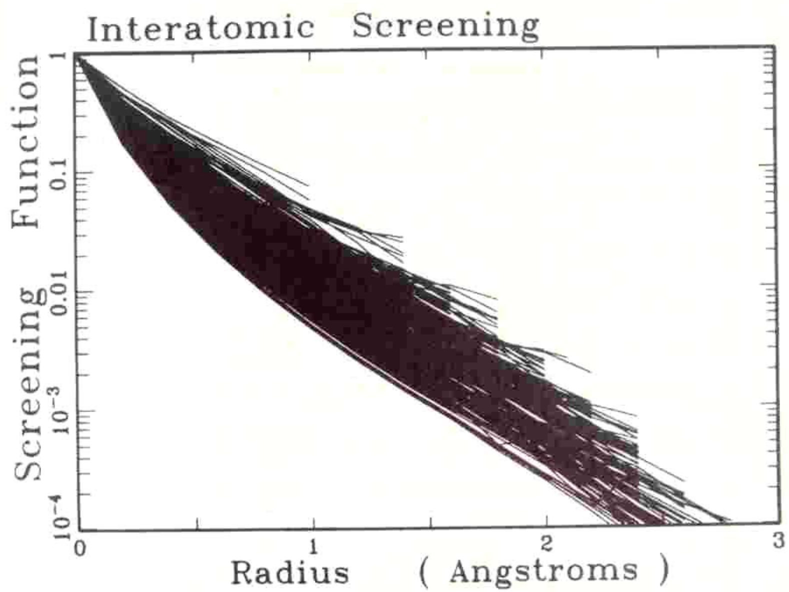


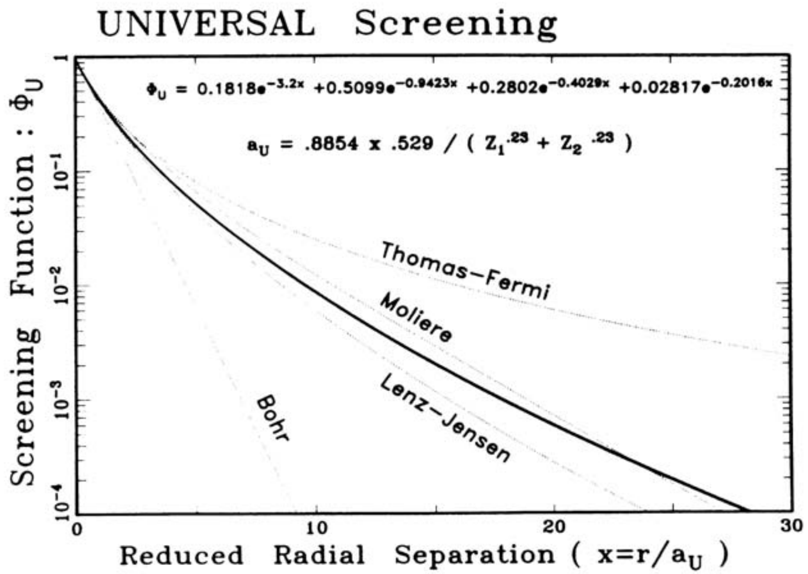
Energy loss of ions in matter

Calculation of nuclear stopping









Energy loss of ions in matter

Calculation of nuclear stopping

From the universal screening function a analytical expression for the nuclear stopping power can be derived

$$\varepsilon_n(E) = \frac{8.462\, Z_1 Z_2 S_n(E_r)}{(M_1 + M_2)(Z_1^{0.23} + Z_2^{0.23})}\ \mathrm{eV\,cm^2/10^{15}\,atoms}$$

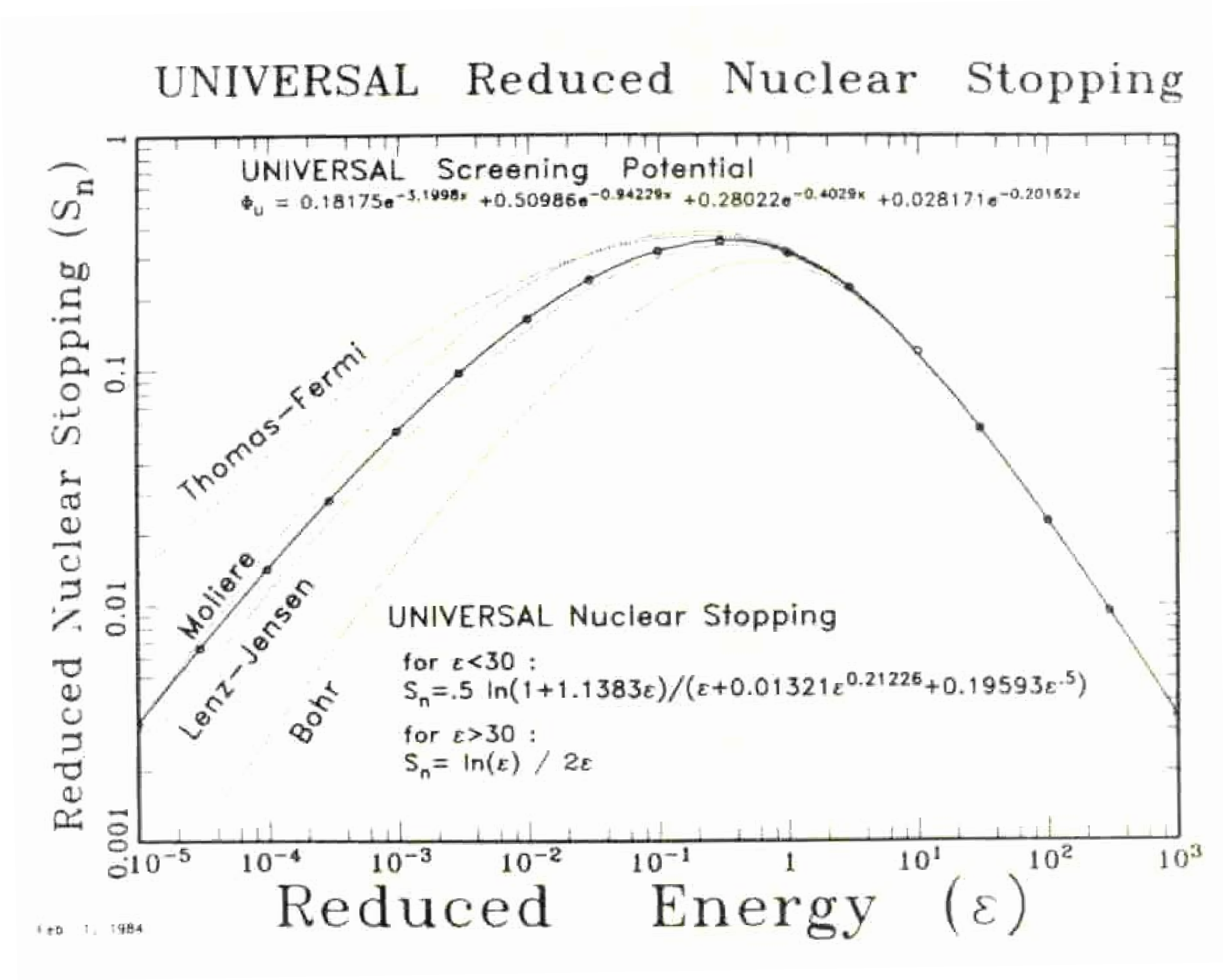
$$E_r = \frac{32.53\, M_2 E}{Z_1 Z_2 (M_1 + M_2)(Z_1^{0.23} + Z_2^{0.23})}$$ is the reduced energy

$$S_n(E_r) = \frac{\ln(1 + 1.1383\, E_r)}{2(E_r + 0.01321\, E_r^{0.21226} + 0.19593\, E_r^{0.5})} \quad \text{for } E_r \le 30\,\mathrm{keV}$$

$$S_n(E_r) = \frac{\ln(E_r)}{2\, E_r} \quad \text{for } E_r > 30\,\mathrm{keV}$$ is the reduced nuclear stopping

Energy loss of ions in matter

Calculation of nuclear stopping



Energy loss of ions in matter

Electronic stopping ε_e From "frictional resistance" of electron clouds

1) Direct kinetic energy transfer to target electrons, mainly e-e collisions
2) Excitation or ionisation of target atoms: promotion of strongly bound target electrons.
3) Excitation of band or conduction electrons: promotion of weakly bound or localised target electrons.
4) Excitation, ionisation, or electron-capture of the projectile.

Low energies: $v \approx 0.1\, v_0$ to $Z_1^{2/3}\, v_0$ LS: $\varepsilon_e \propto v \propto E^{1/2}$

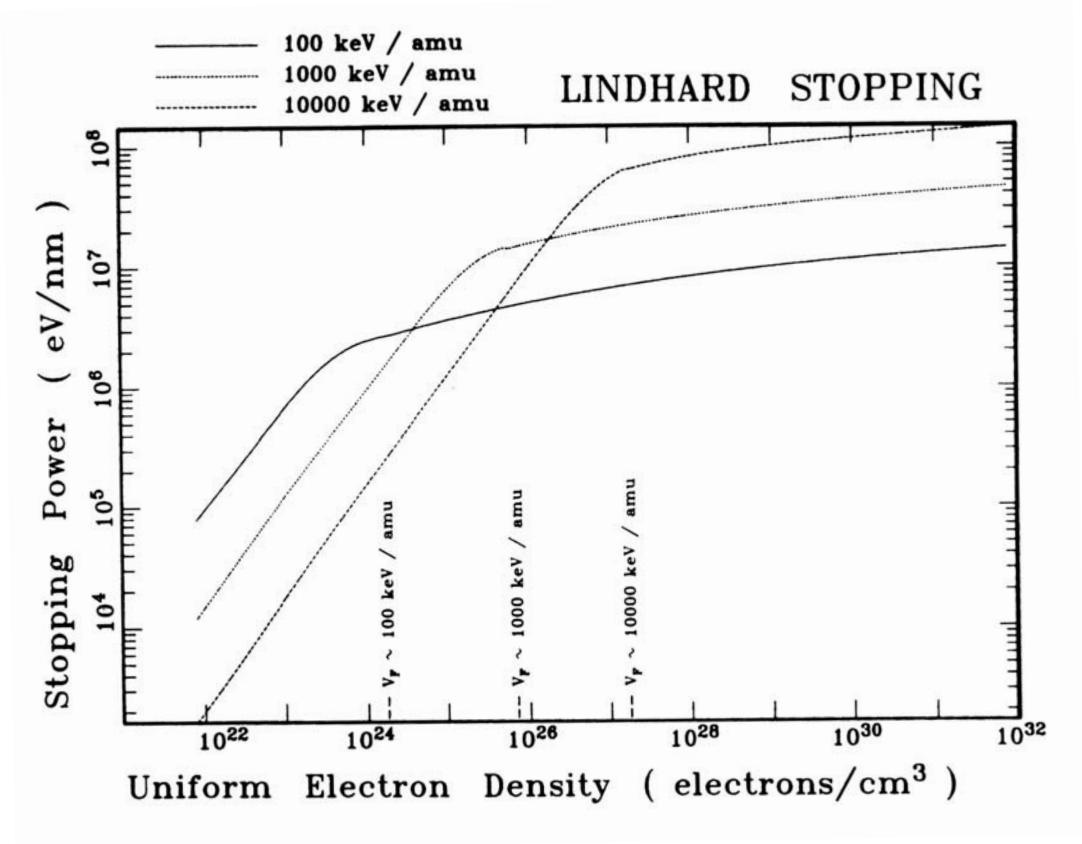
High energies: $v >> v_0$ Bethe-Bloch: $\varepsilon_e = N\, Z_2 \left(Z_1 e^2\right)^2 f(E/\, M_1)$

Intermediate energies: Ion is partially stripped. Effective charge

Energy loss of ions in matter

Low energies

Lindhard-Scharff: non-relativistic many-body self-consistent treatment of a free electron gas at zero temperature and of initial constant density on a fixed uniform positive background, perturbed by a charged particle.



low electron v

high electron v

For a given electron density there is a maximum in ε for a given projectile velocity.

Energy loss of ions in matter

High energies

Bethe-Bloch: Relativistic particle interacting with an isolated atom of harmonic oscillators. First Born approximation. Require that ion velocity be much greater than that of bound electrons (v0).

Intermediate energies

Remember Bethe-Bloch: $\varepsilon_e = N Z_2 (Z_1 e^2)^2 f(E/M_1)$

Use an effective charge $Z_1^*(v, Z_2) = Z_1 \gamma(v, Z_2)$

Heavy ion scaling rule

Projectiles a and b with same velocity in a given medium:

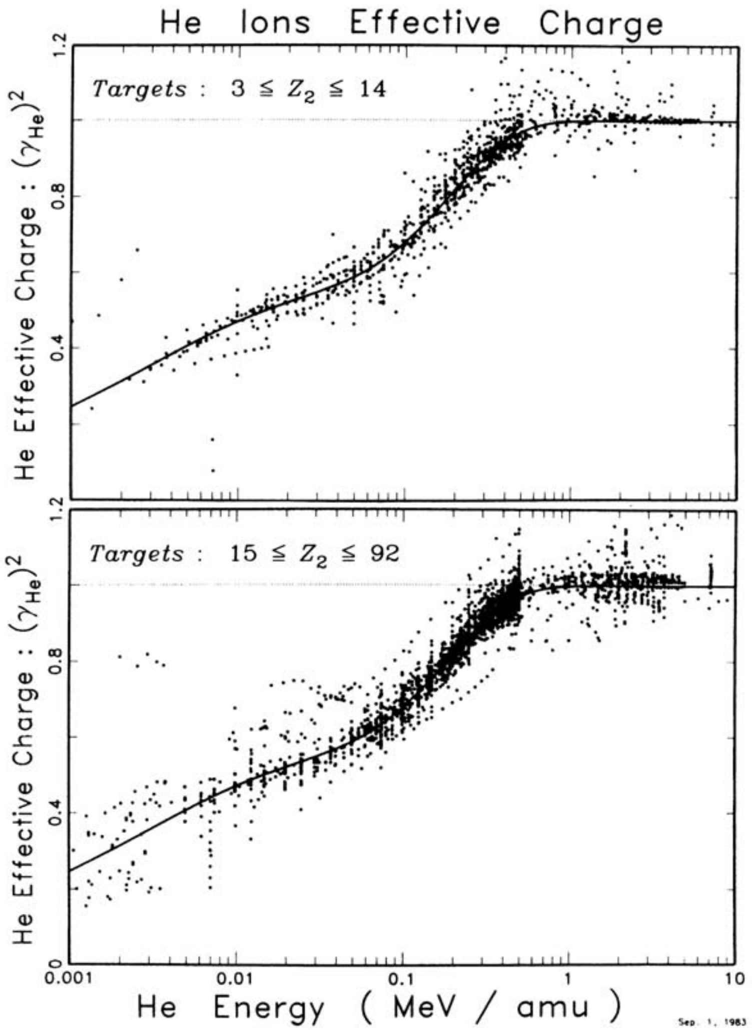
$$\left[\frac{\varepsilon}{(\gamma Z_1)^2}\right]_a = \left[\frac{\varepsilon}{(\gamma Z_1)^2}\right]_b$$

Scale to proton stopping:

$$\varepsilon_{HI} = \varepsilon_H Z_{HI}^2 \gamma_{HI}^2$$

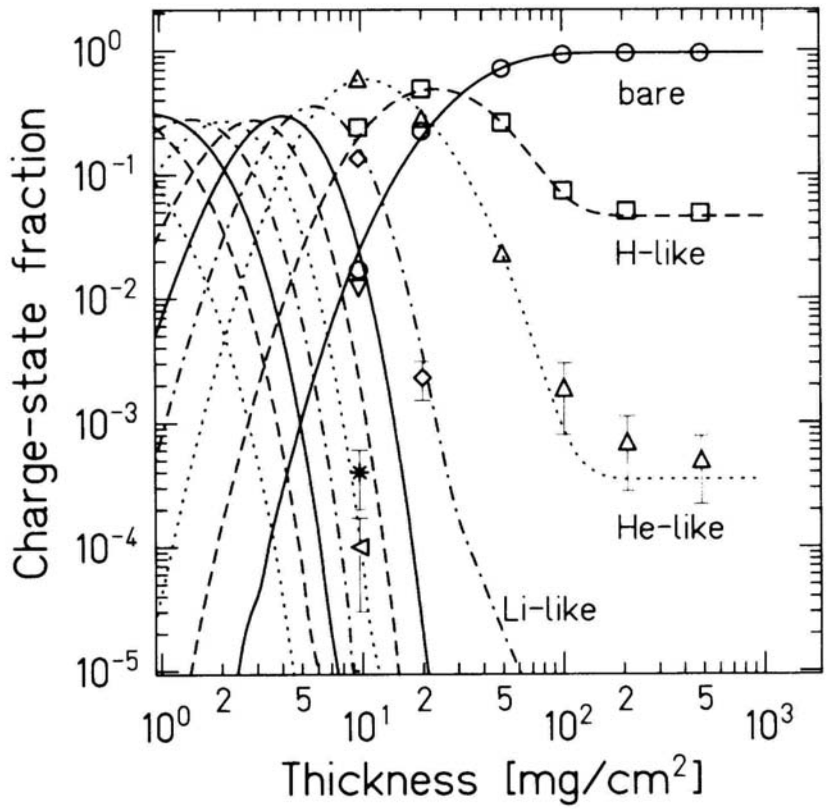
Energy loss of ions in matter

Effective charge

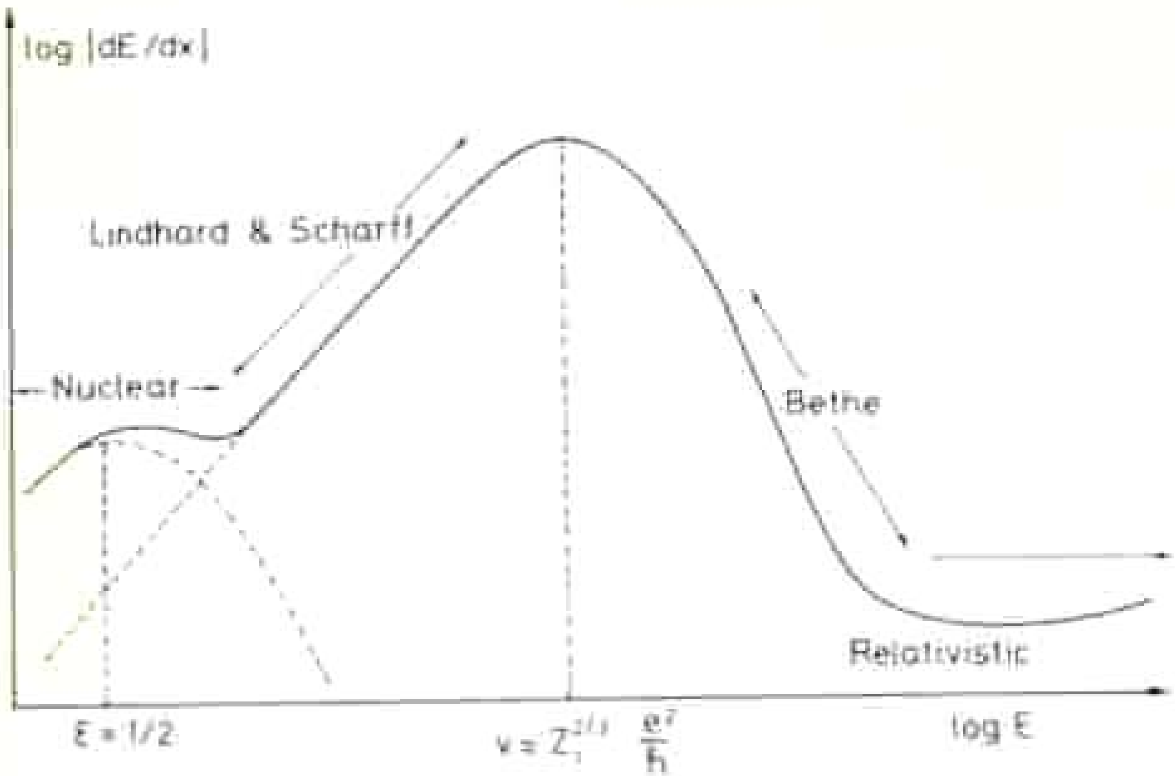


Fit to all He/H data available

1000 MeV/u Au 69+

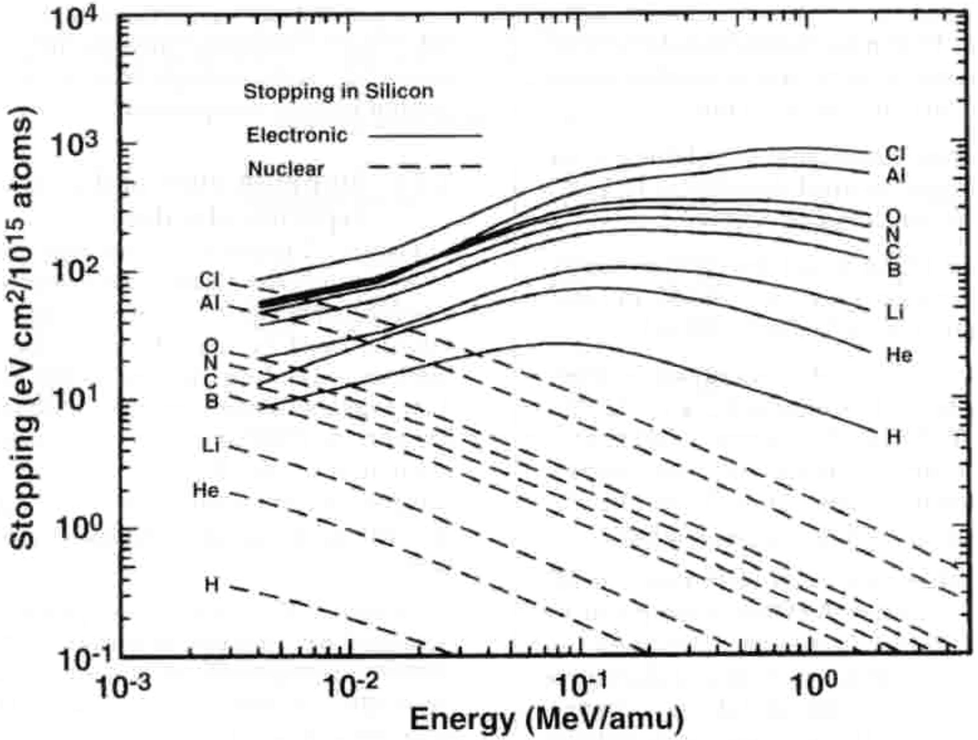


Energy loss of ions in matter

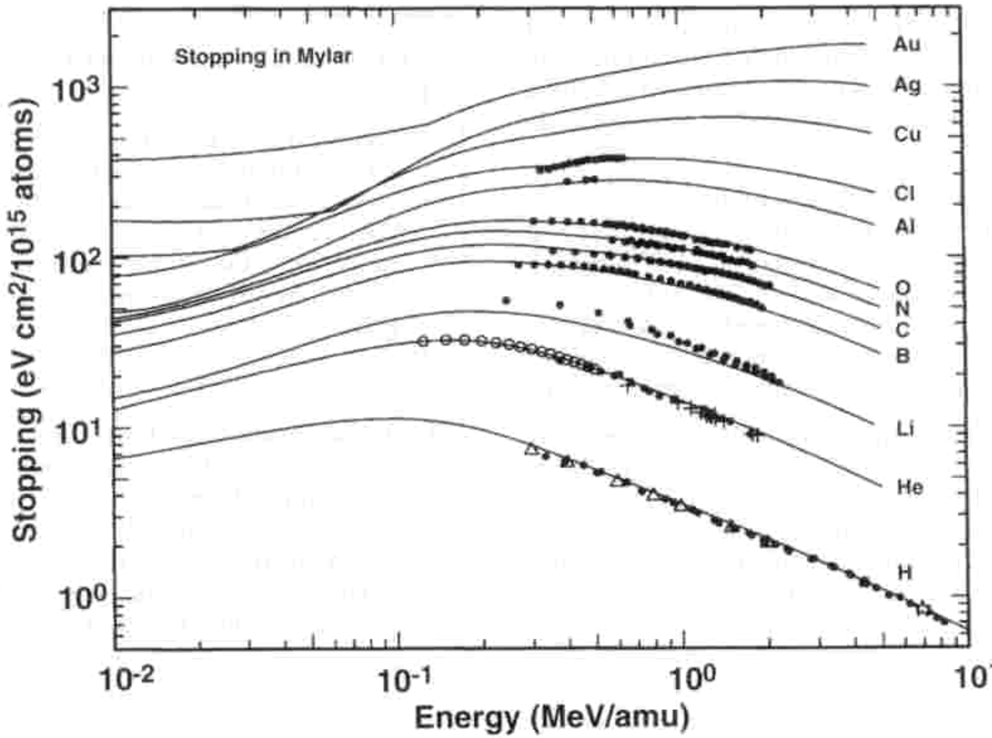


Energy loss of ions in matter

Silicon



Mylar



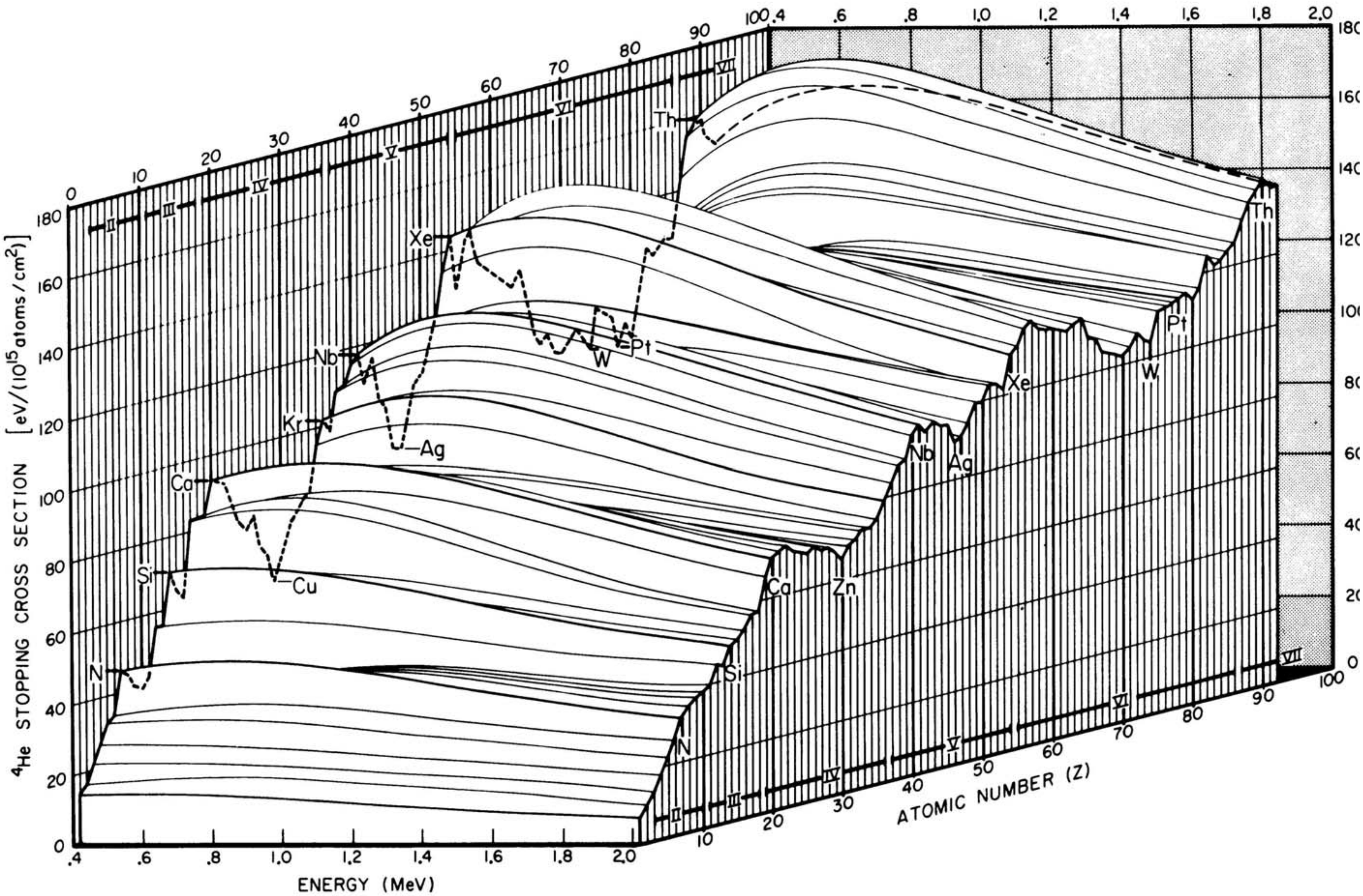
Bragg rule

Chemical effects

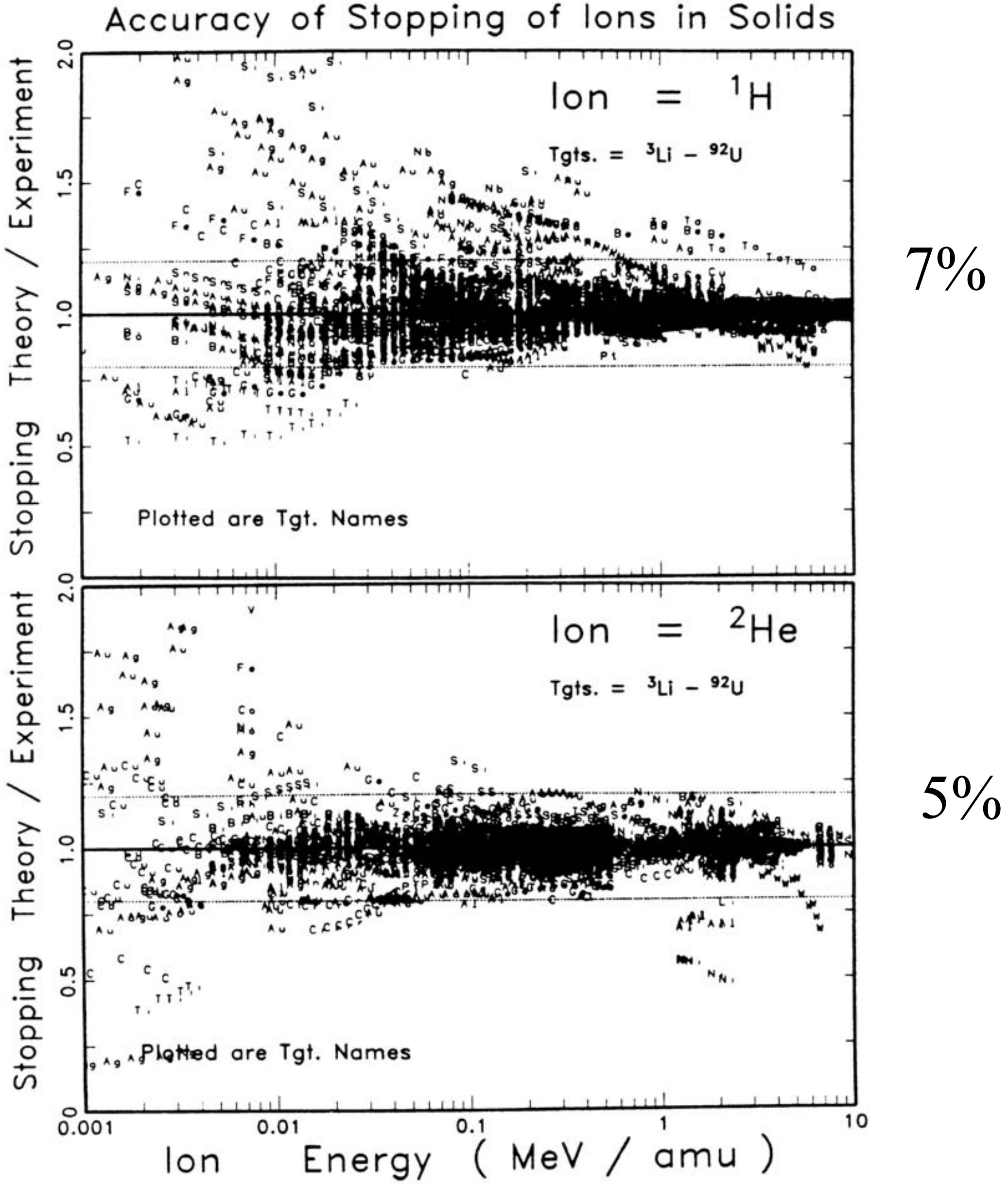
$$\varepsilon^{AB} = m\,\varepsilon^{A} + n\,\varepsilon^{B}$$

$$m + n = 1$$

Energy loss of ions in matter

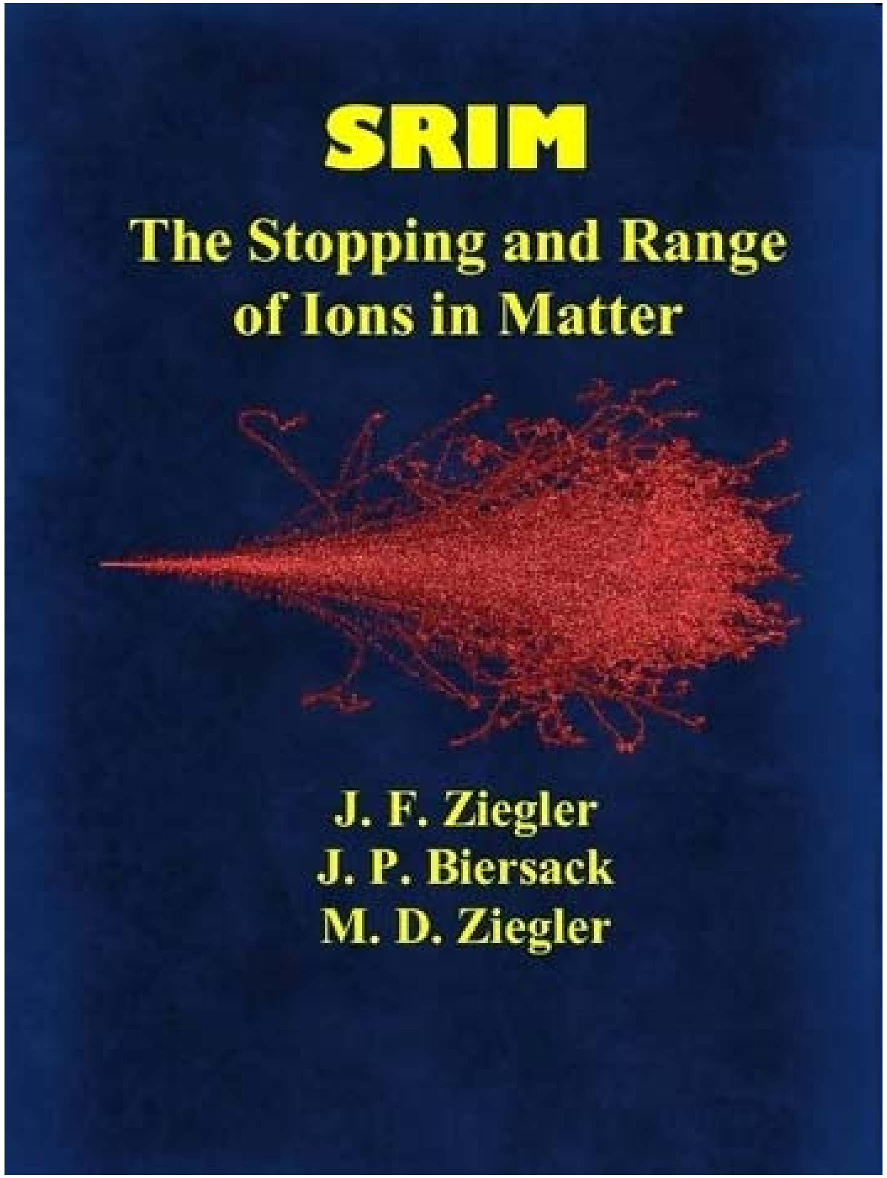


Energy loss of ions in matter



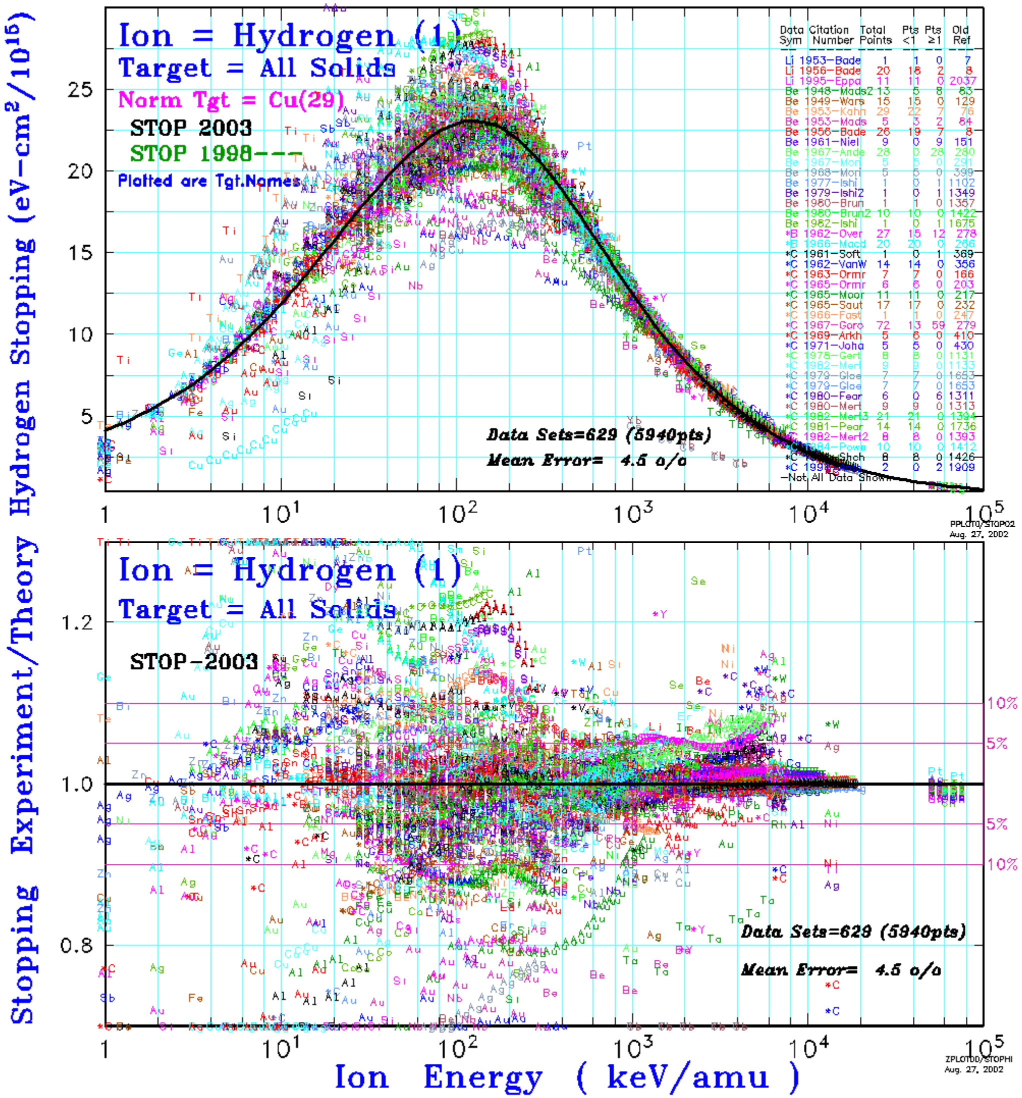
1985. Agreement improved since then!

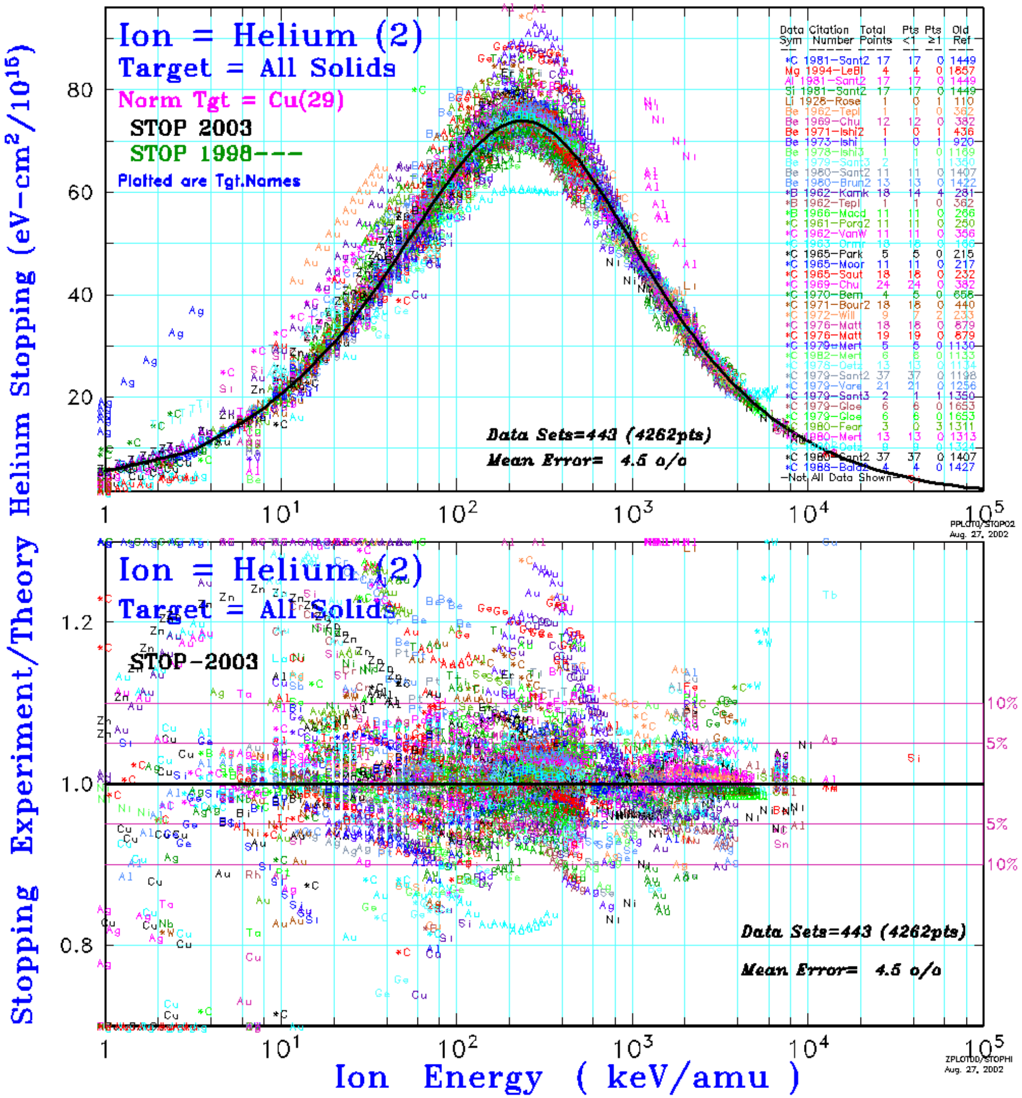
SRIM today www.srim.org



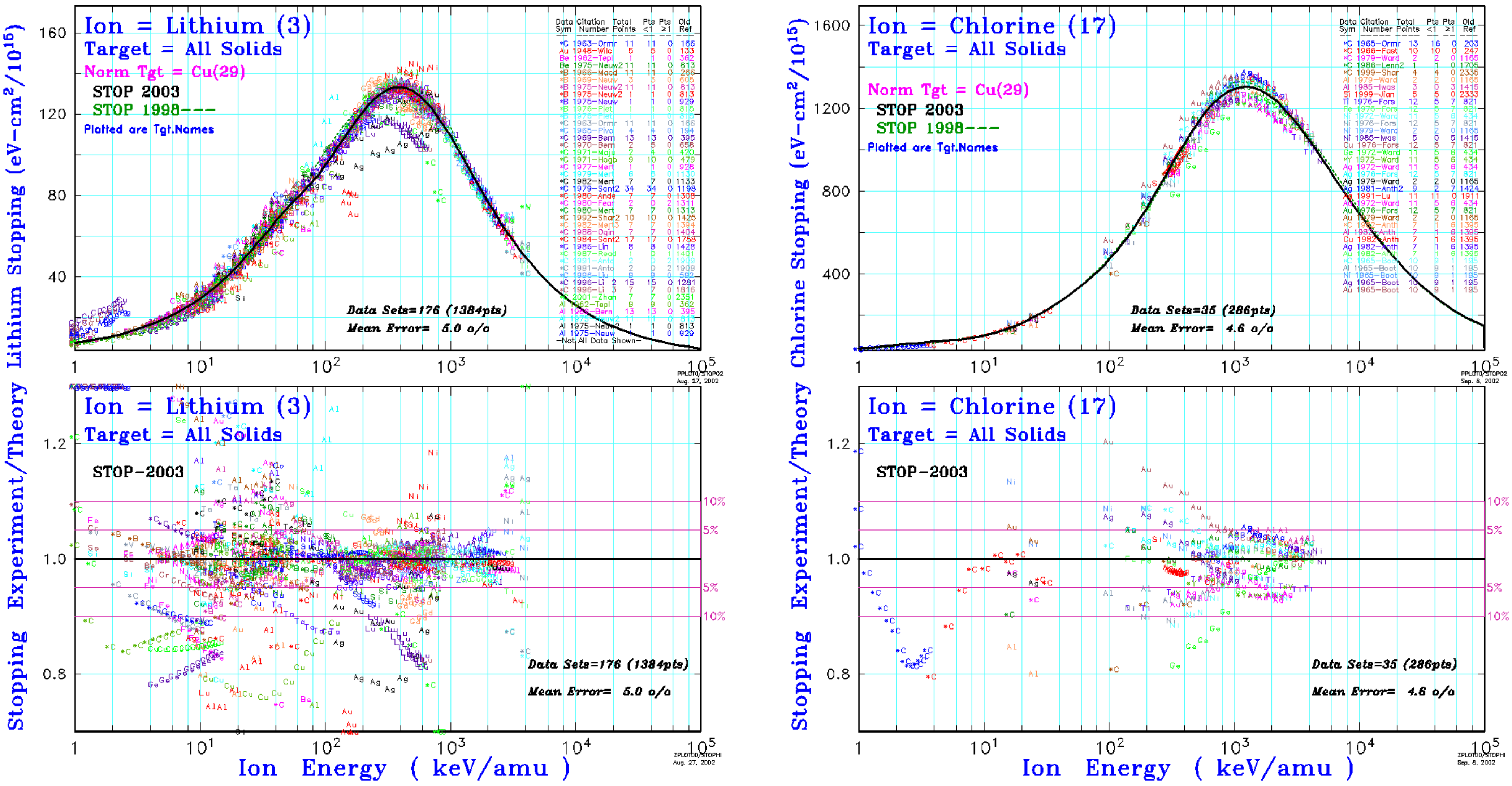
Lulu Press Co. ***http://www.lulu.com/content/1524197***

SRIM today: H and He in everything

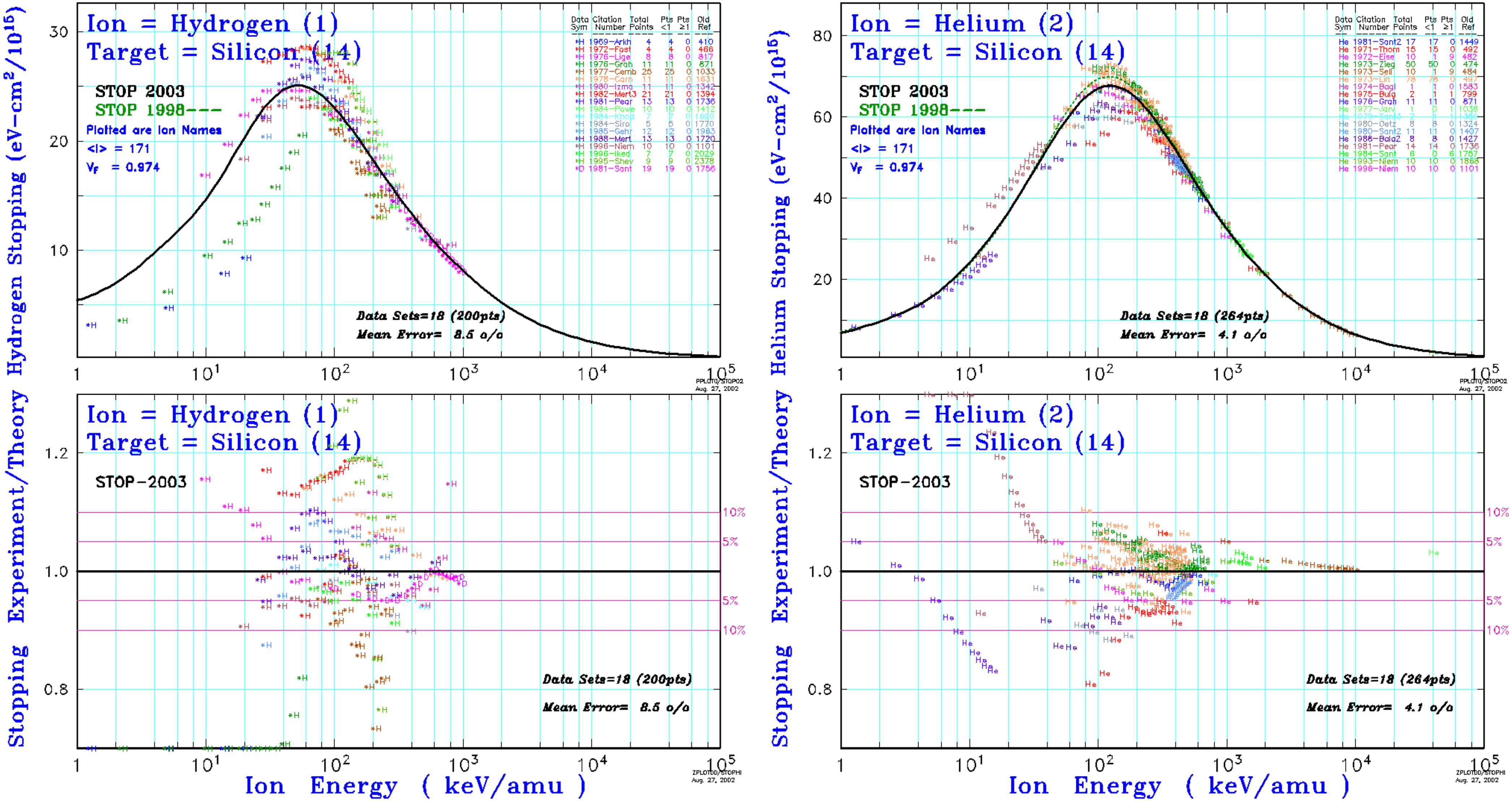




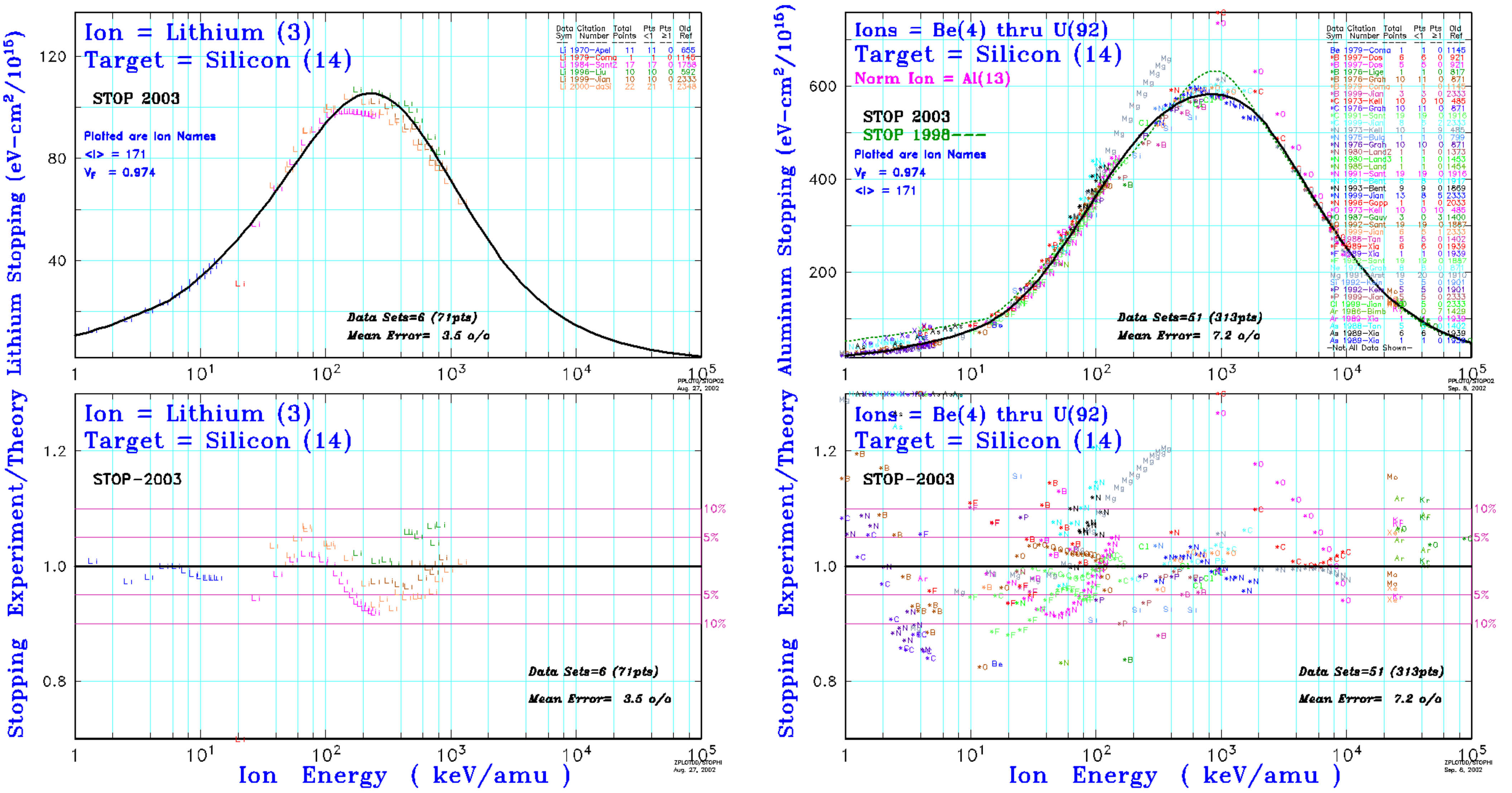
SRIM today: Li and Cl in everything



SRIM today: H and He in Si



SRIM today: Li and HI in Si



Statistical analysis of accuracy

➢ by Helmut Paul: H in solids

Table B1. Mean normalized difference Δ ± σ (in %) for H ions in 17 solid elements
(these are the solid elements covered by ICRU 49)

E/A_1 (MeV)	**0.001 - 0.01**	**0.01 - 0.1**	**0.1 - 1.0**	**1 - 10**	**10 - 100**	**0.001 - 100**
No. of points	207	1272	2393	1156	196	5224
AZ 77	5.5 ± 12	-1.2 ± 12	-3.4 ± 8.3	-1.1 ± 3.9	-0.7 ± 0.6	-1.9 ± 8.9
J 82	11.7 ± 12	2.1 ± 11	-1.1 ± 7.3	-0.9 ± 3.7	-0.2 ± 0.5	0.2 ± 8.4
ZBL 85	-7.0 ± 24	-1.2 ± 12	-3.0 ± 7.8	-0.3 ± 4.2	0.3 ± 2.1	-2.0 ± 9.5
ICRU 49 (p+a star)	5.8 ± 12	0.8 ± 11	-0.7 ± 7.1	-0.2 ± 4.1	0.0 ± 0.5	0.1 ± 7.9
SRIM 2003	4.8 ± 13	0.6 ± 11	-0.9 ± 6.8	-0.6 ± 3.8	-0.1 ± 0.6	-0.2 ± 7.7

Statistical analysis of accuracy

➢ by Helmut Paul: He in solids

Table B3. Mean normalized difference $\Delta \pm \sigma$ (in %) for He ions in 16 elemental solids
(These are the solid elements covered by ICRU 49)

E/A_1 (MeV)	**0 - 0.01**	**0.01 - 0.1**	**0.1 - 1.0**	**1 - 10**	**10 - 100**	**0 - 100**
No. of points	94	942	1610	332	11	2989
Z 77	6.1 ± 25	4.8 ± 8.4	0.5 ± 5.6	0.1 ± 3.3	0.5 ± 1.0	2.0 ± 8.1
ZBL 85	19 ± 24	3.5 ± 8.1	0.7 ± 5.8	-0.5 ± 3.5	0.8 ± 2.4	2.0 ± 8.3
ICRU	4.9 ± 24	2.6 ± 7.9	0.2 ± 5.7	0.5 ± 3.4	0.9 ± 0.9	1.1 ± 7.6
SRIM 2003	10.2 ± 21	3.5 ± 7.8	0.5 ± 5.4	-0.1 ± 3.3	0.2 ± 0.9	1.7 ± 7.3

Statistical analysis of accuracy

➢ by Helmut Paul: H in gases

Table B2. Mean normalized difference $\Delta \pm \sigma$ (in %) for H ions in all elemental gases except F, Cl, Rn						
E/A_1 (MeV)	**0.001 - 0.01**	**0.01 - 0.1**	**0.1 - 1.0**	**1 - 10**	**10 - 100**	**0.001 - 100**
No. of points	116	329	535	303	11	1294
AZ 77	-1.2 ± 6.5	-1.1 ± 5.1	-1.8 ± 4.2	-0.3 ± 2.0	-0.1 ± 0.3	-1.2 ± 4.3
J 82	-1.1 ± 9.4	-0.1 ± 4.6	0.5 ± 3.9	0.9 ± 3.2	3.2 ± 0.6	0.4 ± 4.7
ZBL 85	23 ± 13	22 ± 11	0.4 ± 6.8	-1.1 ± 1.7	-1.0 ± 0.5	7.6 ± 13
ICRU	-0.7 ± 6.5	-1.1 ± 5.0	-1.2 ± 3.7	-0.8 ± 1.6	-0.2 ± 0.5	-1.0 ± 4.1
SRIM 2003	1.7 ± 4.9	-0.1 ± 4.7	-0.4 ± 3.6	-0.2 ± 1.6	0.2 ± 0.3	-0.1 ± 3.8

Statistical analysis of accuracy

➢ by Helmut Paul: He in gases

Table B4. Mean normalized difference $\Delta \pm \sigma$ (in %) for He ions in all elemental gases except F, Cl, Rn

E/A_1 (MeV)	**0 - 0.01**	**0.01 - 0.1**	**0.1 - 1.0**	**1 - 10**	**0 - 10**
No. of points	5	181	669	205	1060
Z 77	-0.5 ± 6.0	-1.6 ± 3.6	1.0 ± 3.3	1.6 ± 2.2	0.7 ± 3.3
ZBL 85	7.2 ± 13	2.6 ± 5.7	3.2 ± 4.3	-0.7 ± 1.5	2.4 ± 4.6
ICRU	0.5 ± 6.8	-1.4 ± 3.5	0.3 ± 3.6	0.5 ± 1.2	0.1 ± 3.3
SRIM 2003	-5.4 ± 6.1	-0.1 ± 3.2	0.3 ± 3.2	-0.2 ± 1.1	0.1 ± 3.0

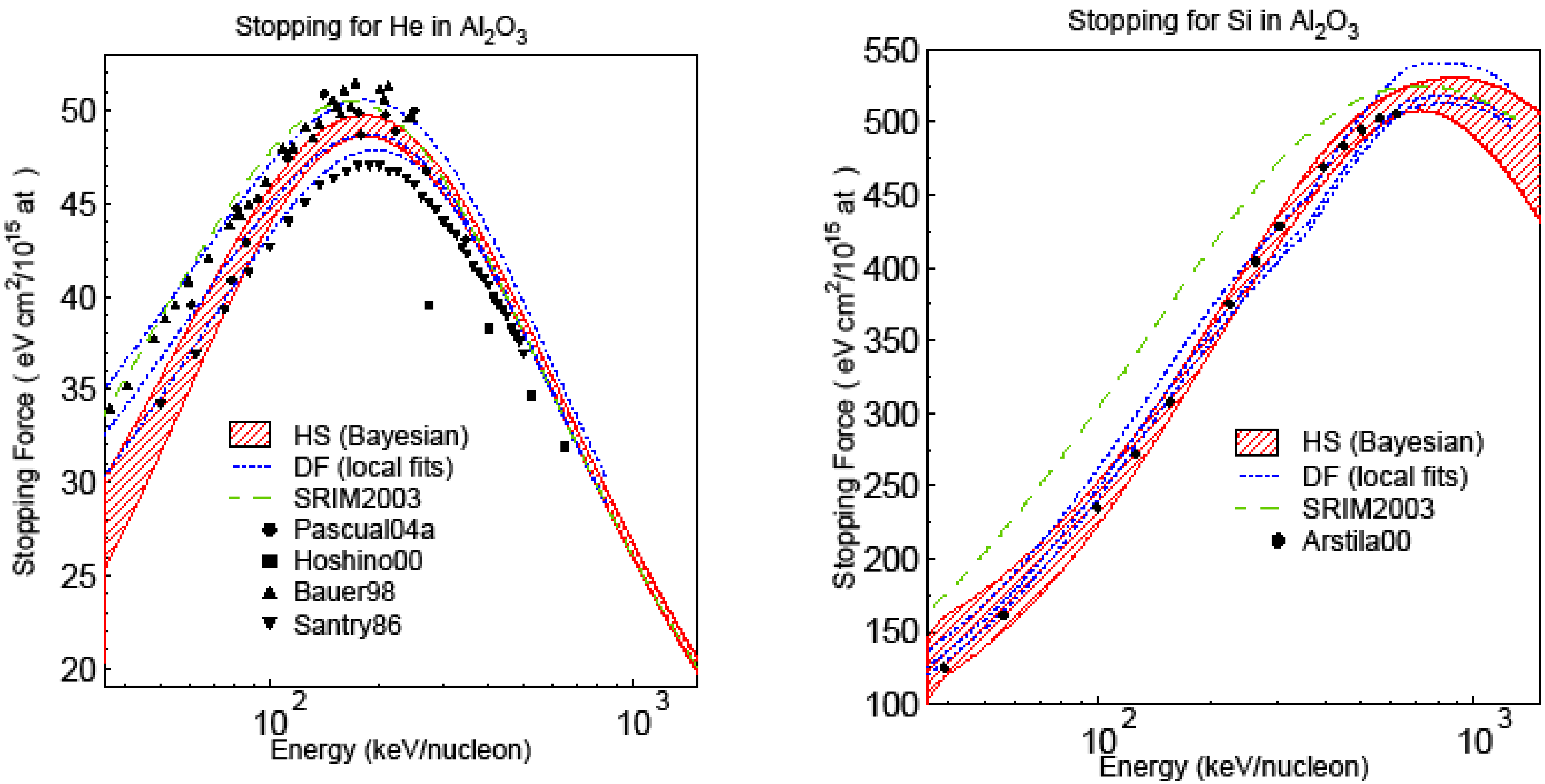
Statistical analysis of accuracy

- by Helmut Paul: HI from Li to Ar in solids

Table D1. Mean normalized difference $\Delta \pm \sigma$ (in %) for ions from $_3$Li to $_{18}$Ar in the elemental solids covered by ICRU 73.

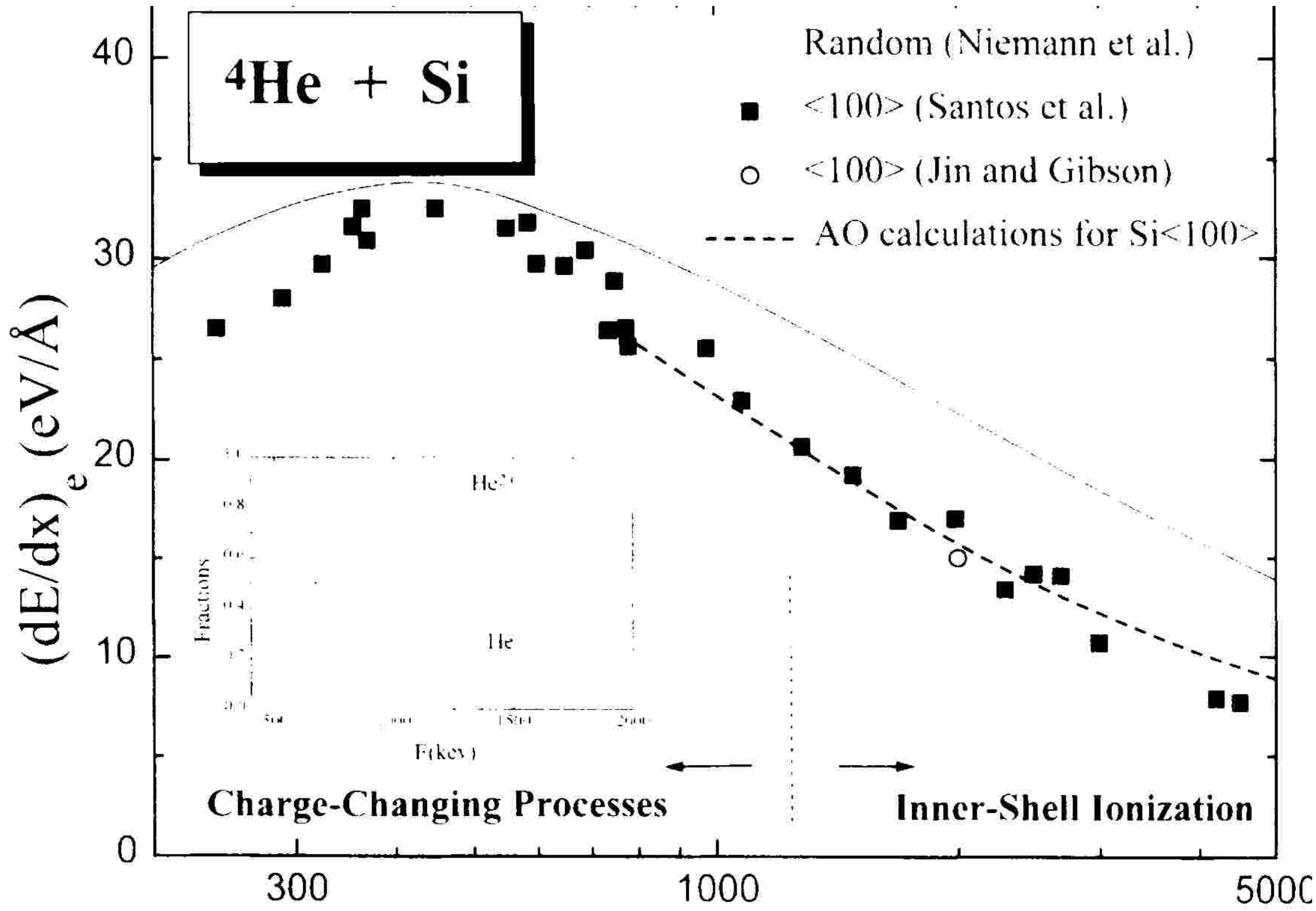
E/A_1 (MeV)	0.025 - 0.1	0.1- 1	1 - 10	10 - 100	100-1000	0.025-1000
No. of points	1399	3452	1262	175	11	6299
MSTAR v.3, mode b	2.5 ± 9.9	0.1 ± 7.3	0.8 ± 5.5	0.1 ± 2.2	0.7 ± 1.4	0.8 ± 7.6
SRIM 2003.26	1.3 ± 9.7	-0.9 ± 7.0	-0.3 ± 5.6	-1.6 ± 2.9	-0.1 ± 1.6	-0.3 ± 7.4
ICRU 73	-11.4 ± 20	-6.8 ± 12	-3.0 ± 6.6	-0.8 ± 3.0	-0.8 ± 1.9	-6.9 ± 13

Stopping in compounds



Energy loss of ions in matter

Channelled stopping



Straggling

Basic concept

The slowing down of a particle beam is accompanied by a spreading of the beam energy, due to statistical fluctuations in the number of collision processes and energy transferred in each one.

Bohr Model

- Distribution is Gaussian when the energy transfers to target electrons in individual collisions are small compared to the width of the energy loss distribution. This fails for thick targets, where the total energy loss during penetration exceeds ≈ 25%.

- In the high velocity limit, the energy loss is dominated by electronic excitations and straggling is almost independent of projectile velocity. In the Gaussian distribution regime Bohr derived for the variance of the average energy loss:

$$\Omega_B^2\,[\mathrm{keV}^2] = 0.26\, Z_1^2\, Z_2\, Nt\,[10^{18}\,\mathrm{at/cm}^2]$$

Straggling

Corrections to Bohr model, other models

Lindhard and Scharff: correction for low ion velocities

$$\frac{\Omega^2}{\Omega_B^2} = \begin{cases} 0.5L(x), \text{ for } E < 75\,Z_2\,[\text{keV/amu}] \\ 1, \text{ for } E \geq 75\,Z_2\,[\text{keV/amu}] \end{cases}$$

$$L(x) = 1.36\,x^{1/2} - 0.016\,x^{3/2},\ x = E[\text{keV/amu}]/(25\,Z_2)$$

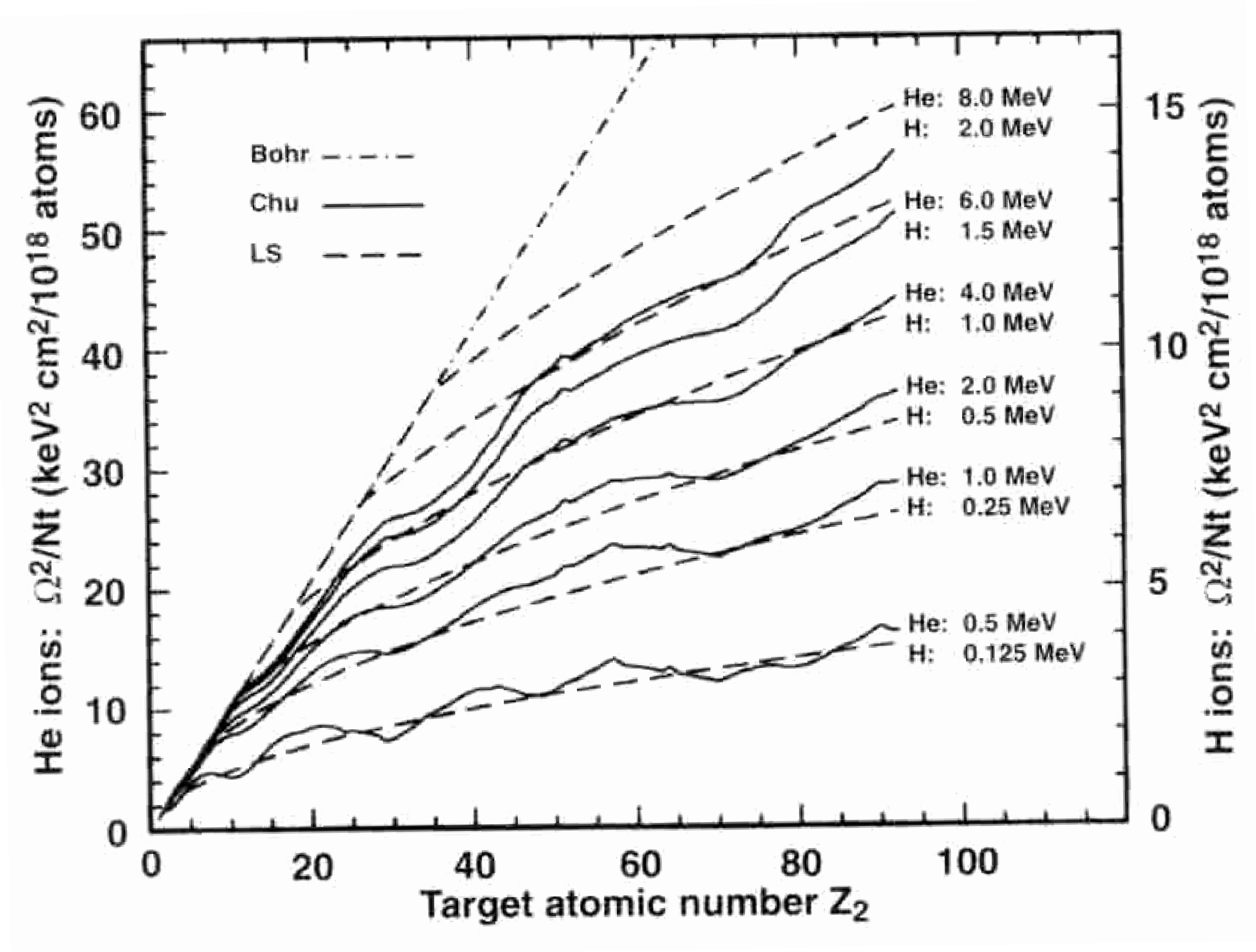
Chu: Hartree-Fock-Slater model of electron density, leads to a further correction to the Bohr model.

Heavy ions: Charge exchange is important. Use Bohr model with Chu correction, plus the effective charge scaling approach, plus correlation effects between nuclear and electronic stopping

Compounds and mixtures: Linear additivity approach

$$\frac{(\Omega^{AB})^2}{N^{AB}\,t} = \frac{m(\Omega^A)^2}{N^A\,t} + \frac{n(\Omega^B)^2}{N^B\,t}$$

Straggling



Calculations for light ions: better than 10%

For heavy ions: 20-30% is often reported

Conclusions

- SRIM is generally fine
- Care is needed for compounds
- Care is needed for heavy ions
- Care is needed even for H and He
- For high accuracy work, need to check the stopping power used!
- May need to use experimental stopping